



Scuola Internazionale Superiore di Studi Avanzati - Trieste

**Ph.D. Course in Geometry and
Mathematical Physics**

Ph.D. Thesis

Mathematics of the Bose Gas in the Thomas-Fermi Regime

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Academic Year 2018-2019

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The present work constitutes the thesis presented by Daniele Dimonte in partial fulfillment of the requirements for the degree of Ph.D in Geometry and Mathematical Physics, of the Scuola Internazionale di Studi Avanzati - SISSA Trieste, with candidate's internal faculty tutor Prof. Ludwik Dąbrowski.

Acknowledgement

When you reach the end of a long path such as the one of a Ph.D, a reflection on its meaning becomes necessary. These last four years of my life were years of changing and transitions, and I am grateful for most of it. A central role in this transition has been the one played by Michele: I want to thank him, I really owe him a lot in my career. He has taught me a lot, both in mathematics and in how to live as a researcher: I am happy I took the chance of working with him five years ago.

During this four years I travelled a lot, I worked for Sissa but often I didn't work *in* Sissa. I will divide my thanks by places.

When first arriving in Sissa, I was lucky enough to profit from the presence of a local “quantum community”. In particular I am grateful for the presence of both prof. Alessandro Michelangeli and prof. Gianfausto Dell’Antonio and for all the activities they managed to organize. Moreover in Sissa the community of Ph.D students made feel at home, and I would like to thank many people there: Alessandro and Raffaele, for being there before me and for me, the other students of my Ph.D course, to share the path (and the pain), Andrea, Giulia, Lucia, Martina and many other, the “physicists”, with whom we never spoke science and only spoke everything else, Carmen, who was there to talk with me in one of the most difficult moments of this Ph.D. Lastly, in Sissa I had two important partners in crime, Giulio and Matteo: we shared offices, discussions, dinners, vacations, stress, kolf and most importantly... Hanabi! I really could have not made it without you two, thank you.

When I wasn't in Sissa I was often in Rome, where Michele worked. There I could gladly benefit from the scientific community, and in particular I would like to thank Sandro Teta, Domenico Finco, Raffaele Carlone (even if not strictly roman) and all the scientific community there. Also there I managed to know the local Ph.D students, and I would like to thank them too, in particular: Giulia, for the nice discussions of life and scattering lengths, Lucrezia, who is now probably fed up with my questions of analysis, Giovanni, the first companion along the way, Ian, who was there to talk important decisions in life - and sometimes doughnut holes, Niels, who canoed with me. Also part of the roman group is Emanuela, and I owe her a lot of thanking: she was there to listen when I thought I needed her, and luckily even when I didn't!

From time to time I would also go to Padova to find Federico: an important thank you goes to him too, a third brother, for spending a lot of time in listening to me and to my neverending meaningless midnight mumbling... Thank you!

Since last November I added a new place to my life of wandering, Bern, and for a good reason. Tina, thank you for supporting me and giving to me more than I could ever give to you. Thank you!

Lastly, I often was in Viterbo, my hometown. When there I was lucky enough to have a friend I could count on: I would like to say thank you to Martina, thank you for being there for me. Last but not least, I would like to thank my parents and my family. They have been supporting (and at times tolerating) me since always and I am really grateful for that.

Notation

Throughout the Thesis we work in *natural units*, with the universal reduced Planck constant \hbar and the mass of the particle m set equal to 1 and $1/2$, respectively.

Moreover, we use Landau notation to denote infinite and infinitesimal quantities; more explicitly, if ϵ is a small parameter,

$$f = \mathcal{O}(g) \iff \text{there exists } C > 0 : |f(\epsilon)| \leq C |g(\epsilon)|, \quad (1)$$

$$f = o(g) \iff \lim_{\epsilon \rightarrow 0} \frac{f(\epsilon)}{g(\epsilon)} = 0, \quad (2)$$

and similarly in the case of a large parameter N .

Analogously, if ϵ is a small parameter, we compare different orders of infinity in the following way:

$$\begin{aligned} f_\epsilon &\gg g_\epsilon, & \text{if } \lim_{\epsilon \rightarrow 0} \frac{f_\epsilon}{g_\epsilon} = +\infty, \\ f_\epsilon &\ll g_\epsilon, & \text{if } g_\epsilon \gg f_\epsilon, \\ f_\epsilon &\approx g_\epsilon, & \text{if } \lim_{\epsilon \rightarrow 0} \frac{f_\epsilon}{g_\epsilon} = C, \text{ with } 0 < c < +\infty, \\ f_\epsilon &\lesssim g_\epsilon, & \text{if } \lim_{\epsilon \rightarrow 0} \frac{f_\epsilon}{g_\epsilon} = C, \text{ with } 0 < c \leq 1, \\ f_\epsilon &\gtrsim g_\epsilon, & \text{if } g_\epsilon \lesssim f_\epsilon, \end{aligned} \quad (3)$$

and similarly for a large parameter N .

Concerning the notation for the norms, if for vectors there will be no ambiguity and $\|\cdot\|$ will always represent the Euclidean norm, for a function f , we will denote with $\|f\|$ its L^2 norm, while $\|f\|_p$ will stand for the corresponding L^p norm, with $p \in [1, 2) \cup (2, +\infty]$. For operators the situation is more involved: $\|A\|$ stands for the operator norm of A , defined as

$$\|A\| := \sup_{\|\psi\|=1} |\langle \psi, A\psi \rangle|. \quad (4)$$

Moreover $\mathfrak{S}_\infty(\mathfrak{h})$ denotes the space of compact operators on a separable Hilbert space \mathfrak{h} . Consider now a positive self-adjoint operator A ; having fixed an orthonormal system $\{e_n\}_{n \in \mathbb{N}}$, we define

$$\text{tr } A := \sum_{n \in \mathbb{N}} \langle e_n, A e_n \rangle. \quad (5)$$

This is not always a finite quantity, and given that for any compact operator A , the operator $|A| := (A^*)^{1/2}$ is a positive, compact, self-adjoint operator, we can consider the following Schatten spaces

$$\mathfrak{S}_p(\mathfrak{h}) := \left\{ A \in \mathfrak{S}_\infty(\mathfrak{h}) : \text{tr} \left[(A^* A)^{\frac{p}{2}} \right] < +\infty \right\}, \quad (6)$$

for $p \in [1, +\infty)$.

In particular, if $A \in \mathfrak{S}_1(\mathfrak{h})$, the following series is absolutely convergent:

$$\mathrm{tr} A := \sum_{n \in \mathbb{N}} \langle e_n, A e_n \rangle. \quad (7)$$

The $\mathfrak{S}_p(\mathfrak{h})$ are also called *Schatten ideals* and satisfy the following two properties:

$$\mathfrak{S}_p(\mathfrak{h}) \subseteq \mathfrak{S}_q(\mathfrak{h}), \quad \forall 1 \leq p \leq q \leq +\infty, \quad (8)$$

$$AB, BA \in \mathfrak{S}_p(\mathfrak{h}), \quad \forall A \in \mathfrak{S}_p(\mathfrak{h}), B \text{ bounded}. \quad (9)$$

In particular, any such space endowed with the corresponding norm $\|A\|_p := \left(\mathrm{tr} \left[(A^* A)^{\frac{p}{2}} \right] \right)^{\frac{1}{p}}$ is a Banach space. When $p = 2$ the corresponding space is an Hilbert space, whose elements are called Hilbert-Schmidt operators. For any $p \in [1, +\infty)$, the following hold true:

$$\|A\|_p := \sup_{B \in \mathfrak{S}_{p'}(\mathfrak{h})} \mathrm{tr} [AB], \quad \text{with } \frac{1}{p} + \frac{1}{p'} = 1, \quad (10)$$

$$\|AB\|_p \leq \|A\|_{pq} \|B\|_{pq'}, \quad \forall q \in [1, +\infty]. \quad (11)$$

During the discussion we will also introduce the notion of partial trace; to do so, consider now the Hilbert space of symmetric states defined as $\mathfrak{h}^{\otimes_s N}$. An orthonormal system for this space is given by

$$\{e_{k_1} \otimes \dots \otimes e_{k_N} : k_j \leq k_{j+1}, k_j \in \mathbb{N}, 1 \leq j < N\} \quad (12)$$

with \otimes representing the symmetric tensor product between two functions. Now we can define the partial trace of an operator $A \in \mathfrak{S}_1(\mathfrak{h}^{\otimes_s N})$ for any $1 \leq l \leq N$ as

$$\mathrm{tr}_{l+1, \dots, N} [A] := \sum_{k_{l+1} \leq \dots \leq k_N, k_j \in \mathbb{N}} \langle e_{k_{l+1}} \otimes \dots \otimes e_{k_N}, A e_{k_{l+1}} \otimes \dots \otimes e_{k_N} \rangle_{l+1, \dots, N} \quad (13)$$

where the inner product is only in the last $N - l$ copies of \mathfrak{h} .

Finally, during the discussion, several constants will appear. Unless differently stated, we write C to denote a generic constant that might be different from line to line, but that will never depend on the parameters in use.

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*“If mathematical thinking is defective,
where are we to find truth and certitude?”*

— D. Hilbert, *On the Infinite*

Introduction

The phenomenon of Bose-Einstein Condensation (BEC) (and its relatively recent experimental realization) has been one of the most relevant discoveries in physics of the past century. Physically speaking, a Bose-Einstein (BE) condensate is realized when a macroscopic fraction of the particles in a quantum gas occupies the same one-particle state, and therefore the gas exhibits quantum properties on a macroscopic scale. The idea that a BE condensate could be realized, at least in the case of non-interacting identical bosons, was initially introduced by Einstein in 1925. After reviewing an article by Bose [B24], he noticed that the techniques used by Bose to derive Planck's law could be applied to derive what he called the quantum theory of an ideal gas. Subsequently, in [E24; E25] he showed that, when considering a gas of non-interacting bosons, there is macroscopic occupation of a one-particle state, and therefore BEC.

The experimental realization of BEC's required seventy years to be achieved. The temperature and the pressure necessary to realize condensation are extremely low, so it was first necessary to develop specific techniques to cool down the gas, first using lasers (*laser cooling*) and subsequently removing the most energetic particles (*evaporative cooling*). With these techniques, in 1995, three different groups (Wieman and Cornell [AEMWC95], Ketterle [DMADDKK95] and Hulet [BSTH95; BSH97]) were able to achieve BEC for the alkali gases of rubidium, sodium and lithium, respectively.

On the other hand, in 1938 the first superfluid properties of Helium ^4He were discovered independently by Allend and Misener [AM38] and Kapitza [K38], and in the same year London [L38] established a connection between superfluidity and BEC. In a superfluid the viscosity is really low, and the intrinsic quantum nature of this state of matter becomes clear if it is put in rotation: indeed, the only way the superfluid can react to the rotation is through the nucleation of *quantized vortices*.

The first semi-rigorous effort at proving BEC in a concrete case was attempted by Bogoliubov [B47] in 1947, but it was the experimental realization of BEC that sparked a renewed interest in a more rigorous derivation;

at the same time, this also stimulated a lot of activity in the study of the Gross-Pitaevskii (GP) equation, which is the effective equation describing the one-particle behaviour of the BE condensate.

The mathematical definition of BEC uses the description of a system in terms of its density matrices. More explicitly, a quantum mechanic system of N particles is described by a complex Hilbert space \mathcal{H}_N , which, together with the self-adjoint Hamiltonian H , encodes the physical properties of the system. A state is represented by an element $\Psi_N \in \mathcal{H}_N$; as usual in quantum mechanics, we can also suppose that Ψ_N is normalized and that Ψ_N is determined up to a multiplicative phase, i.e. Ψ_N and $e^{i\theta}\Psi_N$ represent the same physical state. It turns out that, in order to extract information about one-particle observables (i.e., self-adjoint operators acting only on a single particle), it suffices to consider the so called 1-reduced density matrix $\gamma_{P_{\Psi_N}}^{(1)} := \text{tr}_{2,\dots,N} P_{\Psi_N}$, with P_{Ψ_N} the projector on the state Ψ_N . From the physical point of view, the eigenvalues of $\gamma_{P_{\Psi_N}}^{(1)}$ represent the fraction of particles occupying the corresponding eigenstate. In the case of a classical gas, if one increases the number of particles and the volume, keeping the density of particles constant (the so-called *thermodynamical limit*), then, the number of occupied states increases and the fraction of particle occupying a single state decreases and vanishes in the limit. The phenomenon of BEC, on the opposite, corresponds to the existence, in the thermodynamical limit, of a one-particle state, which is macroscopically occupied. More explicitly, there must be a state $\varphi \in \mathcal{H}_1$ such that $\langle \varphi, \gamma_{P_{\Psi_N}}^{(1)} \varphi \rangle \rightarrow c > 0$ as $N \rightarrow +\infty$.

Proving BEC is a hard problem and the mathematical literature about it is wide. In particular, the physical setting suggests that such a result cannot be proven without additional condition on the physical system. First of all, the symmetry of the system plays a crucial role: already in the work of Einstein, it was crucial to assume that the particles are bosons and not fermions. In particular, the Pauli exclusion principle implies that BEC is not possible in fermionic gases. Moreover, in line with the initial idea of considering non-interacting particles, one typically require the gas to be *dilute*, in agreement with the experimental settings. More explicitly, let a be the scattering length of the pair interaction (i.e., its effective range), and ρ be the density of the particles; then, the limit is called dilute if

$$\rho a^3 \rightarrow 0$$

as $N \rightarrow +\infty$. Notice that, in a model with hard spheres, a represents the radius of a single sphere, therefore ρa^3 can be interpreted as the density of space occupied by the spheres, and the fact that this quantity is small suggests that the spheres are in average very far one from the other.

While dealing with a generic thermodynamic limit is in principle quite hard,

in the literature many specific dilute limits are discussed: the most studied is the GP scaling, in which the pair potential scales as $v_N(\mathbf{x}) = N^2 v(N\mathbf{x})$. In this case, the GP parameter given by $g := Na$, with a the scattering length, is constant, as $N \rightarrow +\infty$, and, as we will see, such a limit is dilute. If φ is the one-particle state on which there is condensation and the system is trapped by a potential U , then φ satisfies the GP equation, the cubic nonlinear equation

$$-\Delta\varphi + U\varphi + 8\pi g |\varphi|^2 \varphi = \mu\varphi.$$

Many results have been proven in the GP limit, both in the stationary and in the dynamical frameworks, and we review them in Chapter 2. However, in several experimental settings, it turns out that a different limit regime is more appropriate: the GP parameter is often very large in experiments, as $N \rightarrow +\infty$. To model this regime, one considers an interacting potential of the form $v_N(\mathbf{x}) := N^{3\beta-1} v(N^\beta \mathbf{x})$, with $\beta \in [0, 1]$. If $\beta = 1$, then the scaling reproduces the GP limit discussed above; on the other hand, if $\beta = 0$, one recovers the famous mean-field scaling.

It is noteworthy that, if $\beta < 1$, the scaling is less singular than the GP one; in this case the GP parameter is equal (to leading order) to the integral of v . To consider a model in which the GP parameter is large as N increases, it is convenient to add a multiplicative constant in front of the potential:

$$v_N(\mathbf{x}) := g_N N^{3\beta-1} v(N^\beta \mathbf{x}),$$

with $g_N \rightarrow +\infty$, as $N \rightarrow +\infty$. If $\beta < 1$, the system is still not too singular and the scattering length is given (again, to leading order) by g_N times the integral of v . In particular, there is a choice of g_N such that the limit is still dilute; this is the so-called Thomas-Fermi (TF) scaling, in analogy to the density theory for large atoms.

It is important to notice that, while in the GP limit the effective equation does not depend on N , this cannot be the case in the TF scaling. Indeed, the kinetic and the trapping terms are subleading compared to the interaction term, so a suitable rescaling is needed. The GP equation in the TF regime can indeed be written as

$$-\Delta\varphi + U\varphi + \frac{1}{\varepsilon^2} |\varphi|^2 \varphi = \mu\varphi,$$

with $\varepsilon = \varepsilon(N)$ a small parameter. This is a useful setting for studying the response of superfluids to rotation from a mathematical point of view, and in particular, the nucleation of quantized vortices.

In our work we study the mathematical derivation of the TF limit. First we look at BEC in the ground state. Starting from a many body Hamiltonian in

the TF regime, in Theorem 3.1.2 we prove that there is BEC in the ground state as long as $\beta < \frac{1}{3}$. In this case, indeed, we are able to prove that the number of particles outside the condensate is vanishing as $N \rightarrow +\infty$. Moreover, we are also able to derive the explicit value for the first order of the ground state energy and prove that it depends only on g_N and on the integral of v in Theorem 3.1.3. Subsequently, we use the so-called Bogoliubov approximation to discuss excitations over the ground state and what we expect as a next-to-leading order approximation for the ground state energy.

The next question is whether BEC is preserved or not by time evolution. We prove in Theorem 4.1.5 that if $\beta < \frac{1}{6}$ and if there is BEC on a state ψ_0 at initial time then BEC is preserved on a state ψ_t which satisfies the time-dependent GP equation (in the TF regime)

$$i\partial_t\psi_t = -\Delta\psi_t + U\psi_t + g_N |\varphi_t|^2 \varphi_t.$$

Although we need some technical assumptions on the solution ψ_t , we are able to provide an explicit rate of convergence towards the solution of the effective problem.



This Thesis is divided in four Chapters and we now briefly outline the content of each one.

- In Chapter 1 we give a general overview of the physics of BEC as a physical motivation for the subsequent study.
- In Chapter 2 we introduce the mathematics of BEC, exposing what is known about BEC in both the stationary and dynamical cases.
- In Chapters 3 and 4 we prove our results about BEC in the TF regime in the stationary and dynamical frameworks respectively.

Physics of Bose-Einstein Condensation

In this Chapter, we present the first physical prediction of Bose-Einstein condensation (BEC) for non-interacting gases which is due to Einstein in 1924. Subsequently, we briefly describe the analogous phenomenon for an interacting dilute gas and give an overview of some physical results about it. This will allow us to point out the relevance of the Thomas-Fermi limit in the physics of Bose-Einstein condensates, in particular in relation to the observation of superfluidity and the appearance of quantized vortices.

1.1 Bose and Einstein's Predictions

Starting from an intuition by Bose contained in a work on the statistics of photons [B24], Einstein in [E24; E25] considered a gas of non-interacting, massive bosons, and concluded that, below a certain temperature, a non-zero fraction of the total number of particles occupies the one-particle state with lowest energy.

More specifically, consider the following many-body quantum Hamiltonian for a non-interacting bosonic gas in a box Λ in d dimensions:

$$H_N^0 := \sum_{j=0}^N \frac{1}{2m} \hat{\mathbf{p}}_j^2 = - \sum_{j=0}^N \frac{\hbar^2}{2m} \nabla_j^2 = \sum_{j=0}^N h_j, \quad (1.1)$$

where $\hat{\mathbf{p}} := -i\hbar\nabla$ is the momentum, m is the mass of one particle and \hbar is the reduced Planck constant.

If the bottom of the spectrum of h is $\inf \sigma(h) = \epsilon_0$, the bosonic ground state energy of the system is at $T = 0$

$$E_0^{\text{bos}} := \inf \left\{ \langle \psi | H_N^0 | \psi \rangle : \psi \in L_s^2(\mathbb{R}^{dN}), \|\psi\| = 1 \right\} \quad (1.2)$$

$$= N\epsilon_0, \quad (1.3)$$

where the bosonic constraint is implemented in the fact that we minimize only on states which are symmetric under exchange of particles. In order to prove this simple fact, it is sufficient to show that the r.h.s. of (1.3) is both an upper and lower bound for E_0^{bos} . The lower bound directly follows from the inequality $h \geq \epsilon_0$, while the upper bound is obtained by computing the expectation value of the state $\psi_0^{\otimes N}$, where $h\psi_0 = \epsilon_0\psi_0$. More in general, whenever we consider an Hamiltonian of the form $H_N^0 + V$ with V symmetric and real, the bottom of the spectrum *not* restricted to symmetric function (if it exists) coincides with the bosonic ground state energy, and moreover, the ground state is symmetric. Therefore, when investigating the ground state of a bosonic system, we can equivalently formulate the ground state problem on the non-symmetric space (see also [LSSY05]).

Consider now a basis of eigenvectors for h , labeled by $p \in \mathbb{N}$, with corresponding energies $\{\epsilon_p\}_{p \in \mathbb{N}}$, $\epsilon_p \leq \epsilon_{p+1}$. We denote by $\{N_p\}_{p \in \mathbb{N}}$ the occupation numbers of the corresponding energy levels, with the total number of particles given by $N = \sum_p N_p$. In the grand canonical ensemble, the average occupation number for bosons is given by

$$N_p = \frac{1}{z^{-1}e^{\epsilon_p/(k_B T)} - 1}, \quad (1.4)$$

where $z := e^{\mu/(k_B T)}$ is the fugacity, μ is the chemical potential fixed by the constraint on the total number of particles, and k_B is the Boltzmann constant.

Consider now the **thermodynamic limit**, i.e., the limit $N \rightarrow +\infty$ with $\rho = N/|\Lambda|$ fixed; given that ϵ_p scales like $|\Lambda|^{-d/2}$ in d dimensions, we can replace the summation over excited states with an integral and, for N large, get

$$N_0 = \frac{1}{z^{-1}e^{\epsilon_0/(k_B T)} - 1}, \quad (1.5)$$

$$N = N_0 + \int_{\epsilon_1}^{\infty} d\epsilon \frac{D(\epsilon)}{z^{-1}e^{\epsilon/(k_B T)} - 1}, \quad (1.6)$$

where $D(\epsilon)$ is the density of the states, i.e. the density of states of energy ϵ that in $d = 3$ is of the form

$$D(\epsilon) := \frac{m^{\frac{3}{2}} |\Lambda|}{\sqrt{2}\pi^2 \hbar^3} \sqrt{\epsilon}. \quad (1.7)$$

Now, for ρ and N fixed, we can write $z = z(\rho, N)$ and $N_0 = N_0(\rho, N)$ as functions of ρ and N using (1.6) and (1.5). Moreover, let $\rho_c(T)$ be defined as

$$\rho_c(T) := \frac{1}{|\Lambda|} \int_0^{+\infty} d\epsilon \frac{D(\epsilon)}{e^{\epsilon/(k_B T)} - 1} \quad (1.8)$$

provided the integral is finite. One can easily realize that this is the case only in $d = 3$ (or larger), so that we can compute

$$\rho_c(T) = \frac{m^{\frac{3}{2}}}{\sqrt{2}\pi^2\hbar^3} \int_0^{+\infty} d\epsilon \frac{\sqrt{\epsilon}}{e^{\epsilon/(k_B T)} - 1} \quad (1.9)$$

$$= \left[\frac{mk_B T}{2\pi\hbar^2} \right]^{\frac{3}{2}} \zeta\left(\frac{3}{2}\right) = \rho \left[\frac{T}{T_c} \right]^{\frac{3}{2}} \quad (1.10)$$

where we set $T_c := \frac{2\pi\hbar^2}{mk_B} \left(\frac{\rho}{\zeta(3/2)} \right)^{2/3}$.

If $\rho_c(T)$ is finite, as in three dimensions, and the temperature is below T_c , then the fraction of excited particles cannot exceed $\rho_c(T)$,

$$\rho_0 \geq \rho \left(1 - \left[\frac{T}{T_c} \right]^{\frac{3}{2}} \right) > 0. \quad (1.11)$$

Hence, as N grows, ρ_0 stays positive and there is a macroscopic number of particles in the one-particle ground state. This is the phenomenon of **Bose-Einstein condensation (BEC)**. Notice that $\frac{2\pi\hbar^2}{mk_B} \zeta(3/2)^{-2/3} \approx 10^{-14} \text{K} \cdot \text{cm}^2$, meaning that, for a density of order $10^{13} - 10^{15} \text{cm}^{-3}$, the temperature required to have BEC is $T_c \approx 10^{-6} - 10^{-4} \text{K}$. In particular, such a temperature is way lower than the one needed to observe quantum phenomena ($10^0 - 10^5 \text{K}$).

The case of the interacting gas is much more complicated, and we postpone the discussion of the mathematical precise definition of BEC to Chapter 2. We discuss first the ground state energy asymptotics of a dilute interacting gas of bosons.

1.2 Ground State Energy of an Interacting Bose Gas

Consider now an interacting Bose gas in a three-dimensional box Λ and fix the system to be in three dimensions. The Hamiltonian is of the form

$$H_N^\Lambda = H_N^0 + \sum_{1 \leq j < k \leq N} v(|\mathbf{x}_j - \mathbf{x}_k|). \quad (1.12)$$

The ground state energy of H_N is

$$E_0(N, \Lambda) := \inf \sigma(H_N^\Lambda). \quad (1.13)$$

Given that $E_0(N, \Lambda)$ is an extensive quantity, when taking the thermodynamic limit, we fix the density ρ and consider the limit of the energy per particle

$$e_0(\rho) := \lim_{N \rightarrow +\infty} \frac{E_0(N, \Lambda)}{N}, \quad (1.14)$$

which depends only on the density¹.

It turns out that the first order of $e_0(\rho)$ in the density ρ can be expressed in terms of the scattering length a of the potential v (see Definition 2.3.3 for a precise definition). More importantly, an hypothesis of diluteness is crucial in order to exclude many-body correlations and be sufficiently close to the non-interacting picture. Physically, this assumption can be cast in form of the condition

$$\rho a^3 \ll 1. \quad (1.15)$$

The first one to derive the first order asymptotics of $e_0(\rho)$ as $\rho \rightarrow 0$ was Lenz in [L29], and the result was later refined in [B47], a seminal paper by Bogoliubov in 1957. Many other authors² worked on the derivation of the next orders of the energy asymptotics during the 60's, and the result was the following expansion:

$$e_0(\rho) = \frac{2\pi\hbar^2}{m} a \rho \left[1 + \frac{128}{15\sqrt{\pi}} (\rho a^3)^{\frac{1}{2}} + 8 \left(\frac{4\pi}{3} - \sqrt{3} \right) (\rho a^3) \log(\rho a^3) + \mathcal{O}(\rho a^3) \right]. \quad (1.16)$$

However, all the works mentioned above provided only heuristic derivations and a rigorous proof of the above formula is still lacking. There are anyway some recent advances that we are going to discuss in Subsection 2.4.1.

1.3 Experimental Results and the Thomas-Fermi Regime

After the theoretical prediction of BEC in 1925, it took around thirty years to have a first experimental realization of a Bose-Einstein (BE) condensate. The main difficulty in achieving condensation in a cloud of bosons was the need to reach a really low density and, more importantly, a very low temperature.

¹Note that we will also consider the energy per volume, in the limit of infinite volume; given that the density is fixed, these two values have the same asymptotics, up to a power of ρ .

²See for example [B57; BS57; HY57; GA59; HP59; W59; LY60; L63; LL64; LS64].

To overcome this difficulty, it was necessary to develop several new techniques. The first step towards achieving BEC was given by the invention of *laser cooling*, which allowed to cool the gas down to temperatures of order 10^{-4}K at an average of 10^9 particles per cm^3 . This was still too high of a temperature, though, and only the development of the technique of *evaporative cooling* allowed to reach even lower temperatures, by removing the most energetic atoms from the cloud. The drawback of this process is however that a large number of atoms are lost, leaving only about $10^4 - 10^7$ atoms in the trap, but at a final temperature below 10^{-6}K . The combination of these techniques allowed several groups to achieve (independently) BEC for different gases of alkali atoms in 1995; Rubidium ^{87}Rb in [AEMWC95], Sodium ^{23}Na in [DMADKK95] and Lithium ^7Li in [BSTH95; BSH97]. Thanks to these results Cornell, Wieman and Ketterle were awarded the 2001 Nobel prize in physics.

Since then, BECs have attracted a lot of attention in theoretical and in experimental physics. From the former point of view much of the theoretical work is based on the study of the **Gross-Pitaevskii (GP) equation**, a non-linear equation in which one of the main parameter is the **GP parameter** $g := Na$, where N is the number of particles and a is the scattering length of the interaction between the particles (for a more precise description of these concepts, we refer to Chapter 2). Mathematically, one often considers a picture in which g is kept constant as N grows, which can be then interpreted as a short range and mean-field regime for a dilute Bose gas. On the other hand, what happens in concrete physical situations is that the GP parameter is actually quite large, as it can be easily deduced by combining the information on the number of particles with the value of the scattering length, tuned, e.g., via a Feshbach resonance mechanism (see for example [BP04; ECHSC03; F01; FZ06; KTU02; L02]). Such a regime is actually better described in what is called the **Thomas-Fermi (TF) limit**, in which the GP parameter is assumed to diverge as $N \rightarrow +\infty$. This becomes even more apparent when considering rotating systems, which is an important setting for BECs due to their superfluidity features: in this limit the effective energy functional is obtained dropping the kinetic contribution to the energy, which then resembles the TF density functional for atoms.

1.3.1 Superfluidity and Quantization of Vortices

An interesting property of BECs is that they often exhibit superfluidity. In order to give a definition of superfluidity, let us first consider a classical fluid: given the mean fluid velocity \mathbf{v} , the vorticity of the fluid is defined as $\boldsymbol{\omega} := \text{curl } \mathbf{v}$. If the fluid rotates around a point at a fixed velocity $\boldsymbol{\Omega}$ (where the convention is that it rotates clockwise with speed $\Omega := |\boldsymbol{\Omega}|$ around the

axis $\Omega^{-1}\Omega$), then it can be considered as a rigid body and its velocity is given by $\mathbf{v} = \Omega \times \mathbf{x}$. In this case the vorticity is constant and $\omega = 2\Omega$. More in general, if the vorticity is non-vanishing, we say that there is a vortex in the fluid.

In the case of a quantum fluid, the velocity field is *irrotational* almost everywhere: indeed, in a superfluid, the state is described by a complex valued function (called in this context *order parameter*) $\psi = e^{i\varphi} |\psi|$ in which the density of the fluid is identified with $\rho = |\psi|^2$ and the velocity is encoded in φ :

$$\mathbf{v} = \frac{\hbar}{m} \nabla \varphi. \quad (1.17)$$

The order parameter satisfy the GP equation

$$i\hbar \partial_t \psi = -\frac{\hbar^2}{2m} \Delta \psi + F(\psi) \psi. \quad (1.18)$$

We note now that equation (1.18) implies that the density ρ satisfy a continuity equation of the form

$$\partial_t \rho + \operatorname{div} \mathbf{j} = 0, \quad (1.19)$$

with the current density \mathbf{j} defined as

$$\mathbf{j} := \frac{\hbar}{2mi} (\bar{\psi} \nabla \psi - \psi \nabla \bar{\psi}). \quad (1.20)$$

Defining the velocity of the fluid through $\mathbf{j} =: \rho \mathbf{v}$, we get (1.17). Given that the state ψ is single-valued, the vorticity is zero as soon as ψ does not vanishes. The **vortices** of the gas now correspond to zeroes of ψ around which there is a nontrivial winding number. To calculate such a topological degree, we evaluate the circulation of the vorticity around a loop containing a vortex: since ψ is the phase of a single-valued function, we immediately deduce that if γ is a loop around a zero of ψ we get

$$\oint_{\gamma} \mathbf{v} \cdot d\mathbf{l} = \frac{\hbar}{m} \oint_{\gamma} \nabla \varphi \cdot d\mathbf{l} \in \frac{h}{m} \mathbb{Z}. \quad (1.21)$$

A typical feature and characteristic mark of superfluidity is precisely the nucleation of quantized vortice. Note indeed that any superfluid with the properties above can store angular momentum only by creating quantized vortices.

Such phenomena have been observed in the experiments using different techniques (see in particular [MAHHW99; MCW00; MCWD00; RBD02;

ARVK01; RAVXK01]). Theoretically, this is justified by the fact that the state ψ of a trapped BE condensate solves the GP equation

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi + \frac{4\pi\hbar^2g}{m}|\psi|^2\psi, \quad (1.22)$$

where $g := Na$ is the previously mentioned GP parameter, and therefore, it might display the superfluid behavior described above.

1.3.2 TF Regime for Rotating BECs

The ground state problem for a superfluid in a rotating frame can be naturally formulated as a variational problem, i.e. we minimize the effective nonlinear energy functional $\mathcal{E}_{\text{phys}}$ conserved by (1.22) under the constraint $\|\psi\| = 1$. In a rotating frame with velocity $\mathbf{\Omega}_{\text{ext}}$, its energy is given by

$$\begin{aligned} \mathcal{E}_{\text{phys}}[\psi] := \int d\mathbf{r} \left\{ \frac{\hbar^2}{2m} |\nabla\psi|^2 + U(\mathbf{r})|\psi|^2 \right. \\ \left. + \bar{\psi} \mathbf{\Omega}_{\text{ext}} \times \mathbf{L} \psi + \frac{2\pi\hbar^2g}{m} |\psi|^4 \right\}, \end{aligned} \quad (1.23)$$

where $\mathbf{L} := \mathbf{r} \times (-i\hbar\nabla)$ is the angular momentum operator. Since there is a preferred direction given by the versor of $\mathbf{\Omega}_{\text{ext}}$, we can set $\mathbf{\Omega}_{\text{ext}} = (0, 0, \Omega_{\text{ext}})$. Moreover, we assume U to be harmonic, i.e.,

$$U(\mathbf{r}) := \frac{m}{2} (\alpha_x^2 x^2 + \alpha_y^2 y^2 + \alpha_z^2 z^2), \quad \text{with } \alpha_* > 0, \quad (1.24)$$

and denote by

$$\ell := \left(\frac{\hbar}{m\alpha_z} \right)^{1/2} \quad (1.25)$$

the characteristic length in the z -direction.

Rescaling all the lengths by ℓ , i.e., setting $\phi(\mathbf{r}) := \ell^{3/2}\psi(\mathbf{r})$, the energy becomes

$$\int d\mathbf{r} \left\{ \frac{1}{2} |\nabla\phi|^2 + \tilde{U}(\mathbf{r})|\phi|^2 + \frac{1}{\alpha_z} \bar{\phi} \mathbf{\Omega}_{\text{ext}} \times \mathbf{L} \phi + \frac{2\pi g}{\ell} |\phi|^4 \right\}, \quad (1.26)$$

where $\tilde{U}(\mathbf{r}) := \frac{1}{2} (\beta_x^2 x^2 + \beta_y^2 y^2 + z^2)$, with $\beta := \alpha_z^{-1}\alpha$. Interestingly enough, if we set

$$\varepsilon := \left(\frac{\ell}{8\pi g} \right)^{\frac{2}{5}}, \quad (1.27)$$

then, using for example the experimental data of the ENS group as in [MCWD00], we get that

$$\varepsilon = 2.75 \cdot 10^{-3} \ll 1 \quad (1.28)$$

is a small parameter.

Given that the value of ϵ is small, one can equivalently consider a scaling of the interacting potential in which the GP parameter $g = Na$ goes to infinity as $N \rightarrow +\infty$. This is the TF limit that we mentioned before.

The study of the minimization problem of the GP equation in the TF limit is interesting on its own and there is a vast literature on the subject (both by numerical experiments [AD15; FJS05; MCW00; MCWD00] and by rigorous analysis [AAB05; CD16; CPHY11; CPHY12; CRY11; CY08; IM061; IM062; R12; SS12]). In particular, one can observe several phase transitions for rotating condensates, as the rotational speed increases. To this purpose it is convenient to rescale the lengths further and set.

$$R := \frac{\ell}{\sqrt{\epsilon}}, \quad u(\mathbf{r}) := R^{\frac{3}{2}} \phi(R\mathbf{r}), \quad \tilde{\Omega} := \frac{1}{\epsilon \alpha_z} \Omega_{\text{ext}}, \quad (1.29)$$

and in this case the energy becomes

$$\int d\mathbf{r} \left\{ \frac{1}{2} |\nabla u|^2 + \bar{u} \tilde{\Omega} \times \mathbf{L} u + \frac{1}{\epsilon^2} \left[\tilde{U}(\mathbf{r}) |u|^2 + \frac{1}{4} |u|^4 \right] \right\}. \quad (1.30)$$

If $\tilde{\Omega} = 0$ the minimizer exists and it is unique (up to a phase), and corresponds to a positive real state. The bulk of the BE condensate (i.e., the area where the mass is asymptotically concentrated as $\epsilon \rightarrow 0$) is a disc centered at the origin. When the system is put under rotation, but $\tilde{\Omega} = \mathcal{O}(1)$, as $\epsilon \rightarrow 0$, then the minimizer is unaffected and does not show any reaction to the rotation. In the laboratory, though, the rotation can be made really fast, so $\tilde{\Omega} \rightarrow +\infty$ as $\epsilon \rightarrow 0$. In particular, there are several phase transitions, as $\tilde{\Omega}$ increases. When $\tilde{\Omega}$ crosses a threshold $\tilde{\Omega}_{c1} \approx |\log \epsilon|$, a first vortex is nucleated in the minimizer, and, as the rotational speed increases, more vortices are nucleated. The bulk however does not change, vortices eventually fill it, distributing as in a lattice-like structure³. A second transition occurs when $\tilde{\Omega}$ crosses a second critical threshold $\tilde{\Omega}_{c2} \approx \epsilon^{-1}$: the centrifugal forces become then comparable with the trapping and, in the case of harmonic trapping, they eventually destroy it. If however, there is some anharmonic trapping, as realized in experiments produced by the ENS group, see [BSSD04; SBOD04], the condensate can be trapped for higher rotational speed. In this case, the bulk of the minimizer assumes the shape of an annulus, and vortices are still present in it. There is a final threshold $\tilde{\Omega}_{c3}$ after which vortices are expelled from the bulk and the condensate behaves as in a giant vortex state, where there are no vortices in the bulk, but a large vorticity seems to be concentrated at the origin.

³More precisely, it has been proven in [CPHY11; CY08] that the measure of vorticity is uniformly distributed after a certain rotational speed, but the fact that the optimal distribution is a (triangular) lattice has yet to be proven (see also [SS12]).

While the study of the minimization problem has been carried on in several frameworks with different trappings, the problem of deriving this effective model starting from the many-body system is still to be fully studied. This Thesis aims at filling precisely this void.

CHAPTER 2

BEC and GP Theory: Mathematical Formulation

In this Chapter, we describe the mathematical framework of BEC in a bosonic system. In particular, we provide the precise mathematical definition of BEC, we discuss the property of diluteness and we give an overview of the results available in literature about BEC and effective theories for dilute systems. We start from the thermodynamic limit of the low density Bose gas, then study the mean-field regime, and finally discuss the Gross-Pitaevskii regime and the Bogoliubov approximation. At the end of the Chapter, we introduce in detail the Thomas-Fermi regime which will be studied throughout the rest of the Thesis.

2.1 Many-Body Bosonic Systems

A quantum system is mathematically described by an Hamiltonian operator defined on an Hilbert space. For a system of N bosonic particles the **Hamiltonian** (or energy) is¹

$$H_N := \sum_{j=1}^N h_j + \sum_{1 \leq j < k \leq N} v_{jk}. \quad (2.1)$$

The description of the system is encoded in the way we choose the Hilbert space and the operators h_j and v_{jk} . In particular, given that we want to consider only bosonic particles, we have to restrict ourselves to symmetric functions, so that the **many-body Hilbert space** is

$$\mathcal{H}_N := \mathfrak{h}^{\otimes_s N} \quad (2.2)$$

while h_j are copies of a one-particle self-adjoint operator h , acting on the j -th copy of \mathfrak{h} , and, similarly, v_{jk} are copies of a self-adjoint (usually multiplication) operator v acting on the j -th and k -th copies of \mathfrak{h} . The choices of h ,

¹We do not take into account three- and more-body interactions for the sake of simplicity, since the corresponding effects are expected to be of lower order.

v and \mathfrak{h} varies depending on the type of system we consider; however, h contains the one-particle information (typically a kinetic term and a trapping potential, if present), while v represents the pair interaction, and is given by the multiplication by a function depending only on the distance between the particles. Finally, \mathfrak{h} is a space of square integrable functions over some measurable set (typically \mathbb{R}^d or the torus Π^d).

A **pure state** of our system is a function $\Psi \in \mathcal{H}_N$. Given a state Ψ and a (self-adjoint) operator A , we denote the expectation of A on Ψ as $\langle A \rangle_\Psi$ and we define it as²

$$\langle A \rangle_\Psi := \langle \Psi, A\Psi \rangle = \text{tr} [AP_\Psi]. \quad (2.3)$$

More in general, a **state** is a positive definite operator $\gamma \in \mathcal{B}(\mathcal{H}_N)$ such that $\gamma \geq 0$ and $\text{tr}[\gamma] = 1$. We denote the space of states on \mathcal{H}_N by \mathfrak{S}_N . Then, for a generic state we denote the expectation value of a self-adjoint operator A by $\langle A \rangle_\gamma$ given as

$$\langle A \rangle_\gamma := \text{tr} [A\gamma]. \quad (2.4)$$

For any state, it is also useful to define its reduced density matrices: given $\gamma \in \mathfrak{S}_N$ and for every $k \leq N$, the **k -reduced density matrix** $\gamma^{(k)}$ is

$$\gamma^{(k)} := \text{tr}_{k+1, \dots, N} [\gamma]. \quad (2.5)$$

Given a pure state Ψ , we denote the corresponding density matrix, i.e. the projection on Ψ , and the k -reduced density matrices as γ_Ψ and $\gamma_\Psi^{(k)}$, respectively. An easy calculation allows us to see that the expectation value of the energy on a pure state can be expressed only in terms of its 1- and 2-reduced density matrices, i.e.

$$\langle H_N \rangle_\Psi = N \text{tr} \left[h\gamma_\Psi^{(1)} \right] + \frac{N(N-1)}{2} \text{tr} \left[v_{12}\gamma_\Psi^{(2)} \right]. \quad (2.6)$$

The above rewriting of the expectation value of the energy suggests that in the determination of the ground state energy of a physical bosonic system, only the 1- and 2-reduced density matrices are relevant. This is true but does not lead to a simplification of the problem. Indeed, the ground state problem

²Recall that $P_\Psi := |\Psi\rangle\langle\Psi|$.

consists in the determination of the energy $E(N)$ and the state Ψ_N so that³

$$E(N) := \inf \{ \langle H_N \rangle_\Psi : \Psi \in \mathcal{H}_N, \|\Psi\| = 1 \} \quad (2.7)$$

$$= \inf \left\{ \frac{N}{2} \operatorname{tr} \left[(h_1 + h_2 + (N-1)v_{12}) \gamma_\Psi^{(2)} \right] : \Psi \in \mathcal{H}_N, \|\Psi\| = 1 \right\} \quad (2.8)$$

$$= \langle H_N \rangle_{\Psi_N}. \quad (2.9)$$

The wave function Ψ_N and the energy $E(N)$ are usually called the ground state and ground state energy of the system, respectively, and, under suitable assumptions (see for example [LL01]) on both h and v , Ψ_N is unique (up to a phase), symmetric and it solves the Schrödinger equation

$$H_N \Psi_N = E(N) \Psi_N, \quad (2.10)$$

at least in weak sense.

Then, the question is whether the infimum in (2.8) can be taken over all density matrices on the two-particle space, i.e. if

$$F = \inf \left\{ \frac{N}{2} \operatorname{tr} [(h_1 + h_2 + (N-1)v_{12}) \gamma] : \gamma \in \mathfrak{S}_2 \right\} \quad (2.11)$$

coincides with $E(N)$.

In general, this is false, which is due to the fact that, in considering only two-particle density matrices, we lose the symmetric structure of the initial many-body state Ψ . This is related to the well-known N -representation problem, i.e. the problem of characterizing the two-particle density matrices obtained as reduced matrices of a many-body bosonic state. The problem is still open, even at the level of the ground state: correlations between particles are indeed often present in the minimizer. What is true, however, is that, in the limit $N \rightarrow +\infty$, the ground state energy can be approximated (at least to leading order) by an effective one-particle description.

2.2 Ground State Energy of Non-Interacting Bosons

We first describe a toy case. Consider a system given by N non-interacting bosonic particles in a box $\Lambda = [-\frac{L}{2}, \frac{L}{2}]^d$. The one-particle Hamiltonian is

³The minimization domain should of course be a subset of the self-adjointness domain of the Hamiltonian H_N , or, more generally, of its quadratic form domain. However, we drop such a specification meaning that any state not in the domain of H_N has energy equal to $+\infty$. This is justified by the positivity assumptions we will make on h and v .

given by $h = -\Delta$, and, by testing on the constant function, we immediately get that the ground state energy and the ground state are explicit and equal to

$$E(N) = 0, \quad \Psi_N \equiv \frac{1}{L^{\frac{Nd}{2}}}. \quad (2.12)$$

In particular, if we set $\phi \equiv \frac{1}{L^{\frac{d}{2}}}$, we can explicitly calculate all the k -reduced density matrices as $\gamma_{\Psi_N}^{(k)} = P_\phi^{\otimes k}$. Moreover, we get that the two-particle density matrix is completely determined by the one-particle density matrix and that $\gamma_{\Psi_N}^{(1)}$ has only one eigenvalue equal to 1.

The most physically relevant limit in this framework is the **thermodynamic limit**, in which both the size of the box and the number of particles increase, keeping fixed the total density $\rho := \frac{N}{L^d}$. The relevant quantity to look at is then the energy per unit volume

$$\epsilon := \lim_{L \rightarrow +\infty} \frac{E(N)}{L^d}. \quad (2.13)$$

In this case, ϵ trivially vanishes, but in general one would like to study the dependence of ϵ on the density ρ . While this is an open problem for generic densities, many results are available in the literature on the *low-density regimes*, i.e. when $\rho \approx 0$.

In order to approximate the ground state energy, it would be helpful to know some information about the structure on the ground state. Unfortunately, both the fact that the two-particle density matrix is completely determined by the one-particle density matrix and the fact that $\gamma_{\Psi_N}^{(1)}$ has only one eigenvalue are in general false. Nevertheless, those facts might be true asymptotically as $N \rightarrow +\infty$, in which case we say that BEC occurs (see below).

2.3 Bose-Einstein Condensation

While the concept of condensation is easier to describe for non-interacting systems as there obviously is macroscopic occupation of the one-particle ground state, in presence of interactions this is in general not true. An equivalent way to look at occupation numbers of one-particle states is then to investigate the eigenvalues of the one-particle density matrix of the ground state Ψ_N ; the spectrum of $\gamma_{\Psi_N}^{(1)}$ is indeed discrete, which allows to define BEC for a many-body system.

Definition 2.3.1. We say that there is **Bose-Einstein condensation** (BEC) in the ground state if $\gamma_{\Psi_N}^{(1)}$ has one (and only one) eigenvalue of order 1 in the limit $N \rightarrow +\infty$. More precisely, there exists a state $\phi \in \mathfrak{h}$ and a constant $c \in (0, 1]$ such that

$$\lim_{N \rightarrow +\infty} \langle \phi, \gamma_{\Psi_N}^{(1)} \phi \rangle = c, \quad (2.14)$$

$$\lim_{N \rightarrow +\infty} \text{tr} \left[\gamma_{\Psi_N}^{(1)} (1 - P_\phi) \right] = 0. \quad (2.15)$$

The value c is the **rate of condensation**, and we say that there is **complete (or 100%) condensation** when $c = 1$.

Notice that in the case of complete condensation the 1-reduced density matrix converges to a rank-one operator, and therefore the following Proposition holds true.

Proposition 2.3.2. The following statements are equivalent:

- (a) There is complete condensation, i.e. $1 - \langle \phi, \gamma_{\Psi_N}^{(1)} \phi \rangle \rightarrow 0$ as $N \rightarrow +\infty$;
- (b) $\gamma_{\Psi_N}^{(1)}$ converges to P_ϕ in the Hilbert-Schmidt norm $\|A\|_2 := \sqrt{\text{tr } A^* A}$;
- (c) $\gamma_{\Psi_N}^{(1)}$ converges to P_ϕ in trace norm $\|A\|_1 := \text{tr } |A|$;
- (d) $\gamma_{\Psi_N}^{(1)}$ converges to P_ϕ in operator norm.

In particular,

$$\frac{1}{2} \left\| \gamma_{\Psi_N}^{(1)} - P_\phi \right\|_2 \leq 1 - \langle \phi, \gamma_{\Psi_N}^{(1)} \phi \rangle \leq \left\| \gamma_{\Psi_N}^{(1)} - P_\phi \right\|_2, \quad (2.16)$$

$$\frac{1}{2} \left\| \gamma_{\Psi_N}^{(1)} - P_\phi \right\|_2 \leq \frac{1}{2} \left\| \gamma_{\Psi_N}^{(1)} - P_\phi \right\|_1 = \left\| \gamma_{\Psi_N}^{(1)} - P_\phi \right\| \leq \left\| \gamma_{\Psi_N}^{(1)} - P_\phi \right\|_2. \quad (2.17)$$

Proof. We start from (a) \Rightarrow (b). The proof easily follows from the properties of the Hilbert-Schmidt norm:

$$\left\| \gamma_{\Psi_N}^{(1)} - P_\phi \right\|_2^2 = \text{tr} \left[\left(\gamma_{\Psi_N}^{(1)} - P_\phi \right)^* \left(\gamma_{\Psi_N}^{(1)} - P_\phi \right) \right] \quad (2.18)$$

$$= \text{tr} \left[\left(\gamma_{\Psi_N}^{(1)} \right)^2 \right] + \text{tr} [P_\phi] - 2 \langle \phi, \gamma_{\Psi_N}^{(1)} \phi \rangle \quad (2.19)$$

$$\leq 2 \left(1 - \langle \phi, \gamma_{\Psi_N}^{(1)} \phi \rangle \right). \quad (2.20)$$

On the other hand, (b) \Rightarrow (a) is trivial.

Let us prove now that (c) \Leftrightarrow (d). We follow a proof from [KP10]. Given that P_ϕ is a rank-one projector, there is at most one negative eigenvalue for $\gamma_{\Psi_N}^{(1)} - P_\phi$. Indeed, while it is clear that the bottom of the spectrum of $\gamma_{\Psi_N}^{(1)} - P_\phi$ denoted by λ_0 is non-positive, using the min-max principle (see [RS78]), we get

$$\inf \left(\sigma \left(\gamma_{\Psi_N}^{(1)} - P_\phi \right) \setminus \{ \lambda_0 \} \right) = \quad (2.21)$$

$$= \sup_{\psi \in \mathfrak{h}, \|\psi\|=1} \inf_{\chi \in \{\psi\}^\perp, \|\chi\|=1} \langle \chi, \left(\gamma_{\Psi_N}^{(1)} - P_\phi \right) \chi \rangle \quad (2.22)$$

$$\geq \inf_{\chi \in \{\phi\}^\perp, \|\chi\|=1} \langle \chi, \left(\gamma_{\Psi_N}^{(1)} - P_\phi \right) \chi \rangle = \inf_{\chi \in \{\phi\}^\perp, \|\chi\|=1} \langle \chi, \gamma_{\Psi_N}^{(1)} \chi \rangle \geq 0. \quad (2.23)$$

Now, $\gamma_{\Psi_N}^{(1)} - P_\phi$ is compact and its spectrum is exactly given by $\lambda_0 \leq 0$ and $\{\lambda_n\}_{n>0}$, with $\lambda_n \geq \lambda_{n+1} \geq 0$. From the fact that $\gamma_{\Psi_N}^{(1)} - P_\phi$ is traceless, we deduce that $|\lambda_0| = -\lambda_0 = \sum_{n>0} \lambda_n$, and therefore $\left\| \gamma_{\Psi_N}^{(1)} - P_\phi \right\| = |\lambda_0|$. On the other hand, computing the trace norm of $\gamma_{\Psi_N}^{(1)} - P_\phi$ we get

$$\left\| \gamma_{\Psi_N}^{(1)} - P_\phi \right\|_1 = \sum_{n \geq 0} |\lambda_n| = -\lambda_0 + \sum_{n \geq 0} \lambda_n = -2\lambda_0 \quad (2.24)$$

$$= 2 \left\| \gamma_{\Psi_N}^{(1)} - P_\phi \right\|. \quad (2.25)$$

To conclude the proof of the Proposition is enough to notice that (c) \Rightarrow (b) \Rightarrow (d), due to standard embeddings between Schatten spaces.

□

We will study the phenomenon of condensation for a particular set of potentials that scale with the number of particles N , typically describing a **dilute gas**. To introduce the mathematical concept of diluteness, we need first to recall the definition of scattering length of a potential.

Definition 2.3.3 (Scattering Length). *Let v be a smooth radial function with compact support in \mathbb{R}^3 . A **zero energy scattering state** is the solution of the following problem.*

$$\begin{cases} -\Delta f + \frac{1}{2}vf = 0, \\ \lim_{|\mathbf{x}| \rightarrow +\infty} f(\mathbf{x}) = 1. \end{cases} \quad (2.26)$$

For any $\mathbf{x} \notin \text{supp } v$, f is harmonic and therefore we can define the **scattering length** of v as the real number $a = a(v)$ such that $f(\mathbf{x}) = 1 - \frac{a}{|\mathbf{x}|}$ for any $\mathbf{x} \notin \text{supp } v$.

Remark 2.3.4. *The scattering length can be interpreted as the effective radius of the interaction. In particular, in the case of hard-core potentials where $v(r) = +\infty$, if $r < a$, and $v(r) = 0$ otherwise, a coincides with the scattering length.*

If we expect condensation in the state ϕ , this means that the density of the particles is approximately given by $\rho := |\phi|^2$, and, following [LSSY05], we can define the **mean density** $\bar{\rho}$ as

$$\bar{\rho} := N \int d\mathbf{x} \rho^2(\mathbf{x}). \quad (2.27)$$

Definition 2.3.5 (Dilute limit). *We say that our system is **dilute** if the mean interparticle distance $\bar{\rho}^{-\frac{1}{3}}$ is much larger than the scattering length, i.e.*

$$a\bar{\rho}^{\frac{1}{3}} \ll 1, \quad \text{as } N \rightarrow +\infty. \quad (2.28)$$

We now specify the limits we are interested in.

2.4 Scaling Limits and Effective Theories

The scaling limits we are going to study are mainly referred to the choice of the interacting potential. For every potential, however, we consider three possible settings for the one-particle Hamiltonian (and the corresponding one-particle Hilbert space).

CASE A: SYSTEM IN A BOX

To describe free particles in a box we consider the Hilbert space $\mathfrak{h} := L^2(\Lambda)$ of complex square integrable functions in a box $\Lambda = [-\frac{L}{2}, \frac{L}{2}]^d$ in d dimensions. The one-particle Hamiltonian is given only by the kinetic term⁴ $-\Delta$ with corresponding domain given by $H_{\text{per}}^2(\Lambda)$, i.e. with periodic boundary conditions.

CASE B: TRAPPED SYSTEM IN \mathbb{R}^d

To study a trapped system we consider the Hilbert space $\mathfrak{h} := L^2(\mathbb{R}^d)$ of square integrable functions in \mathbb{R}^d . The one-particle Hamiltonian is however given by a kinetic term plus a potential, $-\Delta + U$, where U is trapping, i.e. $U \in C^\infty(\mathbb{R}^d)$ and $U(\mathbf{x}) \rightarrow +\infty$ as $|\mathbf{x}| \rightarrow +\infty$. In this case h is meant to be the Friedrichs extension of $-\Delta + U$ defined on the dense set $C_c^\infty(\mathbb{R}^d)$.

CASE C: FREE SYSTEM IN \mathbb{R}^d

The Hilbert space for a free system is $\mathfrak{h} := L^2(\mathbb{R}^d)$. The one-particle Hamiltonian is just the kinetic term $-\Delta$ with domain $H^2(\mathbb{R}^d)$.

⁴We recall that we always choose units such that $\hbar = 1$, $m = \frac{1}{2}$.

2.4.1 Thermodynamic Limit

Before introducing the different scaling regimes, it is important to point out that the most relevant setting one would like to investigate is the THERMODYNAMIC LIMIT: in this setting, one picks N particles in a box of side length L and considers the limit $N \rightarrow +\infty$ with the density $\rho := \frac{N}{L^d}$ kept fixed. The object of study is then the energy per volume as a function of the density. This is actually the hardest version of the problem, and there are currently no results for generic ρ .

If, on the other hand, one assumes the gas to be dilute, the asymptotics of the ground state energy can actually be derived. In [LHY57], Lee, Huang and Yang made the striking observation that the first two orders of the ground state energy per volume should depend only on the scattering length of the interacting potential besides the density ρ . Nevertheless, their proof was not rigorous, and it had taken several years to get a complete proof. However, the upper bound was obtained four years later by Dyson in [D57]. The first key result was then the lower bound proven by Lieb, Seiringer and Yngvason in [LSY00] and refined only in 2019 by Fournais and Solovej in [FS]. The corresponding upper bound was rigorously proven by Erdős, Schlein and Yau in [ESY08] and later refined by Yin and Yau in [YY09].

In the setting we want to focus on, the many-body energy is

$$H_N^{\text{tl}} := \sum_{j=1}^N h_j + \sum_{1 \leq j < k \leq N} v(\mathbf{x}_j - \mathbf{x}_k). \quad (2.29)$$

The ground state energy is an extensive quantity with respect to the volume of the box. Hence, to study a limit of large box with fixed density, we set the number of particle as $N(\rho) = \rho |\Lambda|$ and define the **ground state energy per volume** as

$$\mathfrak{e}(\rho) = \lim_{|\Lambda| \rightarrow +\infty} \frac{1}{|\Lambda|} \inf_{\psi \in \mathcal{H}_{N(\rho)}} \frac{\langle \Psi, H_{N(\rho)}^{\text{tl}} \Psi \rangle}{\|\Psi\|^2}. \quad (2.30)$$

The following theorem is the combination result of [YY09; FS]

Theorem 2.4.1 (Yau, Yin 2009 (\leq), Fournais, Solovej, 2019 (\geq)). *Let $v \in C_c^\infty(\mathbb{R}^3)$ be non-negative and spherically symmetric. Then, in the limit $\rho a^3 \rightarrow 0$,*

$$\mathfrak{e}_0(\rho) = 4\pi\rho^2 a \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o\left(\sqrt{\rho a^3}\right) \right). \quad (2.31)$$

An alternative approach which has been taken in the last twenty years is to consider specific settings by rescaling the interacting potentials in such

a way that the gas is dilute. We focus our next discussion on the following three major ones: the mean-field limit, the Gross-Pitaevskii limit and the Thomas-Fermi limit.

2.4.2 Mean-Field Limit and Hartree Theory

We start from the simplest scaling limit, i.e. the **mean-field limit**. We consider N identical bosons in a box⁵ of length L with an interaction whose intensity scales as the inverse of the particle number, while the support of the interaction remains constant. To avoid any ambiguity in the definition of the interaction, we assume that $v \in C_{\text{per}}^\infty(\Lambda)$, and additionally we assume v to be of positive type, i.e. $\hat{v} \geq 0$. The many-body energy is

$$H_N^{\text{mf}} := \sum_{j=1}^N h_j + \frac{1}{N-1} \sum_{1 \leq j < k \leq N} v(\mathbf{x}_j - \mathbf{x}_k). \quad (2.32)$$

The name mean-field comes from the fact that every particle feels an average potential coming from the other particles given by $\frac{1}{2(N-1)} \sum_{k \neq j} v(\mathbf{x} - \mathbf{x}_k)$, and this justifies the choice of the pre-factor. Notice that we could also have chosen N instead of $N-1$ and the results would not be affected. It is easy to see that under these assumptions the gas is dilute.

Proposition 2.4.2. *The scattering length of the potential $\frac{1}{N-1}v$ satisfies*

$$a\left(\frac{1}{N-1}v\right) = \frac{1}{8\pi(N-1)} \int d\mathbf{x} v(\mathbf{x}) + \mathcal{O}\left(\frac{1}{N^2}\right). \quad (2.33)$$

Furthermore, since the reference one-particle state is the constant wave function, $\bar{\rho} \approx N$ and $\bar{\rho}a^3 \approx N^{-2} \ll 1$, i.e. the gas is dilute.

Proof. Recall that, if f_N is the scattering solution and solves

$$-\Delta f_N + \frac{1}{2(N-1)}v f_N = 0, \quad (2.34)$$

then the scattering length satisfies

$$a = \frac{1}{8\pi(N-1)} \int_{\mathbb{R}^3} d\mathbf{x} v(\mathbf{x}) f_N(\mathbf{x}). \quad (2.35)$$

⁵There is not so much difference in this case between the settings [A](#) and [B](#) and therefore we consider the former one.

We then use the Born approximation to calculate the first order of the scattering length:

$$a_N = \frac{1}{8\pi(N-1)} \int_{\mathbb{R}^3} d\mathbf{x} \, v(\mathbf{x}) f_N(\mathbf{x}) = \frac{1}{8\pi(N-1)} \int_{\mathbb{R}^3} d\mathbf{x} \, v(\mathbf{x}) \quad (2.36)$$

$$- \frac{1}{8\pi(N-1)} \int_{\mathbb{R}^3} d\mathbf{x} \left[(-\Delta) \frac{1}{4\pi|\cdot|} * v \right](\mathbf{x}) (1 - f_N(\mathbf{x})) \quad (2.37)$$

$$= \frac{1}{8\pi(N-1)} \int_{\mathbb{R}^3} d\mathbf{x} \, v(\mathbf{x}) \quad (2.38)$$

$$- \frac{1}{32\pi^2(N-1)} \int_{\mathbb{R}^3} d\mathbf{x} \, \frac{1}{|\cdot|} * v(\mathbf{x}) \Delta f_N(\mathbf{x}) \quad (2.39)$$

$$= \frac{1}{8\pi(N-1)} \int_{\mathbb{R}^3} d\mathbf{x} \, v(\mathbf{x}) \quad (2.40)$$

$$- \frac{1}{64\pi^2(N-1)^2} \int_{\mathbb{R}^6} d\mathbf{x} \, d\mathbf{y} \, \frac{v(\mathbf{x}) v(\mathbf{y}) f_N(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} \quad (2.41)$$

$$= \frac{1}{8\pi(N-1)} \int_{\mathbb{R}^3} d\mathbf{x} \, v(\mathbf{x}) + \mathcal{O}\left(\frac{1}{N^2}\right) \quad (2.42)$$

where we integrated by parts using the explicit form of f_N outside of the support of v and concluded the estimate using the general fact that $0 \leq f_N \leq 1$.

□

We investigate two kind of questions: whether there is condensation in the ground state and whether condensation is preserved by the Schrödinger dynamics.

Condensation in the Ground State

We study the behavior of a minimizer Ψ^{mf} of the following variational problem:

$$E_N^{\text{mf}}(N) := \inf \left\{ \langle H_N^{\text{mf}} \rangle_\Psi : \Psi \in \mathcal{H}_N, \|\Psi\| = 1 \right\}, \quad (2.43)$$

$$E_N^{\text{mf}} = \langle \Psi^{\text{mf}}, H_N^{\text{mf}} \Psi^{\text{mf}} \rangle. \quad (2.44)$$

By standard arguments the minimizer exists and is unique.

In order to figure out the expression of the effective model, we first test the functional on a factorized state $\Psi_T := \phi^{\otimes N}$:

$$\frac{1}{N} \langle \Psi_T, H_N^{\text{mf}} \Psi_T \rangle = \int_{\Lambda} d\mathbf{x} \left\{ |\nabla \phi(\mathbf{x})|^2 + \frac{1}{2} v * |\phi|^2(\mathbf{x}) |\phi(\mathbf{x})|^2 \right\} \quad (2.45)$$

$$=: \mathcal{E}^H[\phi]. \quad (2.46)$$

We recall here that the convolution $f * g$ is defined as

$$(f * g)(\mathbf{x}) := \int_{\mathbb{R}^d} d\mathbf{y} f(\mathbf{x} - \mathbf{y}) g(\mathbf{y}). \quad (2.47)$$

This definition applies also to periodic functions, so that $v * |\phi|^2$ is a periodic function, whenever v is. The minimization problem for \mathcal{E}^H is easy to solve.

Proposition 2.4.3. *Let $v \in C_{\text{per}}(\Lambda)$. If we define E^H and ϕ^H as in*

$$E^H := \inf \{ \mathcal{E}^H[\phi] : \phi \in \mathfrak{h}, \|\phi\| = 1 \} = \mathcal{E}^H[\phi^H], \quad (2.48)$$

then, the minimizer is unique up to a phase and

$$E^H = \frac{1}{2|\Lambda|} \int_{\Lambda} d\mathbf{x} v(\mathbf{x}), \quad \phi^H = \frac{1}{\sqrt{|\Lambda|}}. \quad (2.49)$$

Proof. Using $\frac{1}{\sqrt{|\Lambda|}}$ as a trial state we obviously get that (2.49) is an upper bound to E^H . On the other hand,

$$\begin{aligned} \frac{1}{2} \int_{\Lambda} d\mathbf{x} (v * |\phi|^2)(\mathbf{x}) |\phi(\mathbf{x})|^2 &= \frac{\sqrt{|\Lambda|}}{2} \sum_{\mathbf{p} \in \Lambda^*} \widehat{v}(\mathbf{p}) \left| \widehat{|\phi|^2}(\mathbf{p}) \right|^2 \\ &\geq \frac{\sqrt{|\Lambda|}}{2} \widehat{v}(\mathbf{0}) \left| \widehat{|\phi|^2}(\mathbf{0}) \right|^2 = \frac{1}{2|\Lambda|} \int_{\Lambda} d\mathbf{x} v(\mathbf{x}). \end{aligned} \quad (2.50)$$

By uniqueness of the minimizer, we then get that $\phi^H \equiv \frac{1}{\sqrt{|\Lambda|}}$.

□

In order to prove BEC in the mean-field limit, we first have to show that the Hartree functional captures the first order of the energy. Next one proves that the ground state of the many-body problem exhibits condensation on ϕ^H . In the following Theorem we state exactly this result. We omit the proof that can be found in [S11; GS13] in Cases A and B respectively.

Theorem 2.4.4 (Seiringer, 2011/Grec, Seiringer, 2013). *Suppose that $\Psi \in \mathcal{H}_N$ satisfies*

$$\langle H_N^{\text{mf}} \rangle_{\Psi} \leq E_N^{\text{mf}} + \zeta, \quad \text{with } \zeta > 0, \quad (2.51)$$

then

$$\left| \langle \phi^H, \gamma_{\Psi}^{(1)} \phi^H \rangle \right| \leq \frac{C}{N} (\zeta + 1). \quad (2.52)$$

Furthermore there is complete BEC on the state ϕ^H and

$$-C|\Lambda|^{\frac{3}{2}} \leq E_N^{\text{mf}} - \frac{N}{2} \widehat{v}(0) \leq 0. \quad (2.53)$$

In [LNR14] Lewin, Nam and Rougerie proved a similar result but for a larger class of potentials, exploiting the quantum De Finetti theorem. In [Piz1; Piz2; Piz3] Pizzo was able to approximate the minimizer to any order using a multi-scale technique and a Feshbach-Schur flow.

Evolution of a Condensate

We proved that there is complete BEC in the ground state, so we now want to know if condensation is preserved by time evolution. In order to verify it, we consider as initial datum a condensate state generated in a given trap in \mathbb{R}^d and then study condensation as time goes on, after the trap is removed. The interesting result is that BEC is preserved on a timescale of order $\log N$.

There are various results in literature about this problem, see for example [ES07; ESY071; FK09; RS09]. Nevertheless, in [P11] Pickl proved a first general result with weaker hypotheses on the interaction and with explicit bounds on the rate of convergence. We recall here only this last result; the proof relies on the study of the function

$$\alpha(\Psi, \phi) := 1 - \langle \Psi, P_\phi \Psi \rangle, \quad (2.54)$$

where ϕ is the condensate wave function at initial time.

Let Ψ_t^{mf} be the solution of the **many-body Schrödinger equation**

$$\begin{cases} i\partial_t \Psi_t^{\text{mf}} = H_N^{\text{mf}} \Psi_t^{\text{mf}}, \\ \Psi_t^{\text{mf}}|_{t=0} = \Psi_0^{\text{mf}}. \end{cases} \quad (2.55)$$

A solution of the Cauchy problem exists only if Ψ_0^{mf} is in the domain of H_N^{mf} ; for any initial datum not in such a domain, we set $\Psi_t^{\text{mf}} := e^{-iH_N^{\text{mf}}t} \Psi_0^{\text{mf}}$.

Analogously, we define the effective one-body time evolution via the Hartree equation, i.e.

$$\begin{cases} i\partial_t \phi_t^{\text{H}} = -\Delta \phi_t^{\text{H}} + \frac{1}{2}v * |\phi_t^{\text{H}}|^2 \phi_t^{\text{H}}, \\ \phi_t^{\text{H}}|_{t=0} = \phi_0^{\text{H}}. \end{cases} \quad (2.56)$$

We pick the initial datum in the energy domain, so that a weak solution always exists.

Theorem 2.4.5 (Pickl, 2011). *It exists a constant $C > 0$, such that, for any fixed time $t > 0$,*

$$\alpha(\Psi_t^{\text{mf}}, \phi_t^{\text{H}}) \leq e^{Ct} \alpha(\Psi_0^{\text{mf}}, \phi_0^{\text{H}}) + \frac{1}{N} (e^{Ct} - 1). \quad (2.57)$$

Furthermore, if there is BEC in the initial datum, then condensation is preserved for any $t > 0$.

2.4.3 Gross-Pitaevskii Limit

The **Gross-Pitaevskii (GP) Limit** describes N identical bosons in a box of side length L in three dimensions with an interacting potential that in the limit becomes a hard-core potential with short range. The Gross-Pitaevskii limit owes its name to Gross and Pitaevskii who firstly derived (respectively in [G61] and in [P61]) the equation that bears their name and we will see later. The Hamiltonian is written as

$$H_N^{\text{GP}} := \sum_{j=1}^N h_j + N^2 \sum_{1 \leq j < k \leq N} v(N(\mathbf{x}_j - \mathbf{x}_k)). \quad (2.58)$$

In order to figure out the form of the effective energy let us compute again the energy of a factorized state $\Psi_T = \phi^{\otimes N}$:

$$\langle \Psi_T, H_N^{\text{GP}} \Psi_T \rangle \quad (2.59)$$

$$\begin{aligned} &= N \int_{\Lambda} d\mathbf{x} \{ |\nabla \phi(\mathbf{x})|^2 \} \\ &\quad + \frac{N-1}{2} \int_{\Lambda \times \Lambda} d\mathbf{x} d\mathbf{y} N^3 v(N(\mathbf{x} - \mathbf{y})) |\phi(\mathbf{x})|^2 |\phi(\mathbf{y})|^2 \end{aligned} \quad (2.60)$$

$$\approx N \int_{\Lambda} d\mathbf{x} \{ |\nabla \phi(\mathbf{x})|^2 + c |\phi(\mathbf{x})|^4 \} \quad (2.61)$$

with c the integral of v . This guess is however wrong, because even if the energy is quartic in $|\phi|$, the constant c actually differs from the integral of v and is in fact proportional to the scattering length of the potential. Indeed, if we denote by a the scattering length of the unscaled potential v , the effective energy reads

$$\mathcal{E}^{\text{GP}}[\phi] := \int_{\Lambda} d\mathbf{x} \{ |\nabla \phi(\mathbf{x})|^2 + 4\pi a |\phi(\mathbf{x})|^4 \} \quad (2.62)$$

Note that in this case the gas is diluted too, as we can see in the following Proposition.

Proposition 2.4.6. *In the Gross-Pitaevskii limit the gas is dilute. Indeed $\bar{\rho} \approx N$ and the scattering length of the potential satisfies*

$$a(N^2 v(N(\cdot))) = \frac{1}{N} a(v), \quad (2.63)$$

so that $\bar{\rho} a^3 \approx N^{-2} \ll 1$.

To prove the previous Proposition we need some information about the minimization problem for E^{GP} . We state then a Proposition analogous to Proposition 2.4.3.

Proposition 2.4.7. *Let $a \geq 0$ and let E^{GP} and ϕ^{GP} as in*

$$E^{\text{GP}} := \inf \{ \mathcal{E}^{\text{GP}}[\phi] : \phi \in \mathfrak{h}, \|\phi\| = 1 \} = \mathcal{E}^{\text{GP}}[\phi^{\text{GP}}]. \quad (2.64)$$

Then, the minimizer is unique up to a phase and

$$E^{\text{GP}} = \frac{4\pi a}{|\Lambda|}, \quad \phi^{\text{GP}} = \frac{1}{\sqrt{|\Lambda|}}. \quad (2.65)$$

Proof. We proceed as in 2.4.3 and test on the constant function to get that $E^{\text{GP}} \leq \frac{4\pi a}{|\Lambda|}$. On the other hand we have that $\|\phi\|_2 \leq \sqrt[4]{|\Lambda|} \|\phi\|_4$, and therefore $E^{\text{GP}} \geq \frac{4\pi a}{|\Lambda|}$. □

Proof of Proposition 2.4.6. In the GP limit the scattering solution f_N solves

$$-\Delta f_N + \frac{N^2}{2} v(N\mathbf{x}) f_N = 0. \quad (2.66)$$

If we now define $g(\mathbf{y}) := f_N(\frac{\mathbf{y}}{N})$, we get that g solves

$$-\Delta g + \frac{1}{2} v(\mathbf{y}) g = 0, \quad (2.67)$$

which does not depend on N anymore. Moreover the scattering length of the potential v satisfies

$$a(v) = \frac{1}{8\pi} \int_{\mathbb{R}^3} d\mathbf{y} \, v(\mathbf{y}) g(\mathbf{y}). \quad (2.68)$$

Therefore, we get

$$a(N^2 v(N\cdot)) = \frac{N^2}{8\pi} \int_{\mathbb{R}^3} d\mathbf{x} \, v(N\mathbf{x}) f_N(\mathbf{x}) \quad (2.69)$$

$$= \frac{1}{8\pi N} \int_{\mathbb{R}^3} d\mathbf{y} \, v(\mathbf{y}) g(\mathbf{y}) \quad (2.70)$$

$$= \frac{1}{N} a(v). \quad (2.71)$$

Given that ϕ^{GP} is the constant function, $\bar{\rho} = N$ and $\bar{\rho} a^3 \approx N^{-2}$. □

Condensation in the Ground State

The first problem addressed and solved⁶ by Lieb, Seiringer and Yngvason in [LY98; LSY00] was the convergence of the many-body energy to the effective one. This result was achieved applying an old idea by Dyson (see [D57]) of substituting the singular potential with a less singular one, sacrificing some kinetic energy and, at the same time, considering the problem in smaller reduced boxes. The result has recently been proven again by Nam, Rougerie and Seiringer in [NRS16] with different techniques. We present here the original statement contained in [LY98; LSY00].

Theorem 2.4.8 (Lieb, Seiringer, Yngvason, 2001). *Let E_N^{GP} be the ground state energy of the system*

$$E_N^{\text{GP}} := \inf \{ \langle H_N^{\text{GP}} \rangle_\Psi : \Psi \in \mathcal{H}_N, \|\Psi\| = 1 \} \quad (2.72)$$

$$= \inf \sigma(H_N^{\text{GP}}), \quad (2.73)$$

then, E_N^{GP} satisfies

$$\lim_{N \rightarrow +\infty} \frac{E_N^{\text{GP}}}{N} = E^{\text{GP}}. \quad (2.74)$$

The first proof of BEC was obtained few years later by Lieb and Seiringer in [LS02] and by Lieb, Seiringer, Solovej and Yngvason in [LSSY05] for the dilute and trapped gas, respectively. It took almost twenty years then to refine such results and provide information about the fine structure of the minimizer. Indeed the ground state can not be well approximated by a factorized state, but correlations on a suitable scale are present. The result we present here was proven by Boccato, Brennecke, Cenatiempo and Schlein and it is contained in [BBCS18; BBCS2].

Theorem 2.4.9 (Boccato, Brennecke, Cenatiempo, Schlein, 2018). *Let $\Psi \in \mathcal{H}_N$ be such that*

$$\langle H_N^{\text{GP}} \rangle_\Psi \leq E_N^{\text{GP}} + \zeta, \quad \text{for some } \zeta > 0, \quad (2.75)$$

then

$$\left| \langle \phi^{\text{GP}}, \gamma_\Psi^{(1)} \phi^{\text{GP}} \rangle \right| \leq \frac{C}{N} (\zeta + 1). \quad (2.76)$$

Furthermore, in Case A, there is complete BEC in the state ϕ^{GP} and

$$-C |\Lambda|^{\frac{3}{2}} \leq E_N^{\text{mf}} - \frac{N}{2} \hat{v}(0) \leq 0. \quad (2.77)$$

⁶In [LY98] the authors actually consider the thermodynamic limit at low density.

Evolution of a Condensate

The question of whether BEC is preserved in time in the Gross-Pitaevskii limit is more subtle than in the mean-field scaling. After the interesting result proven in one-dimension in [ABGT04; AGT07], a complete answer to the question was given between 2006 and 2010 in a series of paper by Erdős, Schlein and Yau [ESY06; ESY071; ESY072; ESY10], which proved convergence of all the reduced density matrices to projectors onto copies of the one-particle state evolved via the GP equation. However this was only achieved in [Case C](#) and with no quantitative estimates on the rate of convergence. A similar result was proven by Pickl in 2015 in [P15] with completely different techniques (analogous to the one used in [P11]). The same year Fock space techniques combined with the analysis of correlations introduced in [ESY10] allowed Benedikter, De Oliveira and Schlein in [BOS15] to prove explicit error estimates. Such result was then strengthened by Brennecke and Schlein in [BS19] in 2019.

As before, we set $\Psi_t^{\text{GP}} := e^{-iH_N^{\text{GP}}} \Psi_0^{\text{GP}}$, while the **GP evolution** is defined through the following Cauchy problem

$$\begin{cases} i\partial_t \phi_t^{\text{GP}} = -\Delta \phi_t^{\text{GP}} + 8\pi a(v) |\phi_t^{\text{GP}}|^2 \phi_t^{\text{GP}} \\ \phi_t^{\text{GP}}|_{t=0} = \phi_0^{\text{GP}}. \end{cases} \quad (2.78)$$

The main result of [BS19] is the following.

Theorem 2.4.10 (Brennecke, Schlein, 2019). *Let $\phi_0^{\text{GP}} = \phi^{\text{GP}}$ (with ϕ^{GP} defined in Proposition 2.4.7) and the initial datum Ψ_0^{GP} satisfy*

$$\alpha_N := 1 - \langle \phi^{\text{GP}}, \gamma_{\Psi_0^{\text{GP}}}^{(1)} \phi^{\text{GP}} \rangle \rightarrow 0, \quad (2.79)$$

$$\beta_N := \left| \frac{1}{N} \langle \Psi_0^{\text{GP}}, H_N^{\text{GP}} \Psi_0^{\text{GP}} \rangle - E^{\text{GP}} \right| \rightarrow 0. \quad (2.80)$$

Then, there exists a constant $C > 0$ such that

$$1 - \langle \phi_t^{\text{GP}}, \gamma_{\Psi_t^{\text{GP}}}^{(1)} \phi_t^{\text{GP}} \rangle \leq C \left(\alpha_N + \beta_N + \frac{1}{N} \right) e^{Ce^{Ct}}. \quad (2.81)$$

Furthermore, if there is complete BEC at time $t = 0$, then condensation is preserved at any $t > 0$.

2.4.4 Bogoliubov Theory

In the previous sections we stated what is known about the ground state and the ground state energy of many-body bosonic systems. We have seen that

one can characterize the leading order term of the energy and wave function asymptotics as $N \rightarrow +\infty$. The next natural question to ask is whether one can capture the next order approximation of the ground state and how to extend the results to excited states.

We recall that the Hamiltonian H_N can be also seen as a restriction to a single sector of a Fock space Hamiltonian \mathbb{H} . Let us briefly discuss some properties of operators over Fock spaces before proceeding further.

More explicitly, let \mathcal{F}_N be the **bosonic Fock space** defined as

$$\mathcal{F}_N := \bigoplus_{n \geq 0} \mathfrak{h}^{\otimes_s n}. \quad (2.82)$$

For any fixed $f \in \mathfrak{h}$ and for any $\Psi \in \mathcal{F}_N$ we can define the **annihilation operator** $a(f)$ as

$$(a(f) \Psi)^{(n)} := \sqrt{n+1} \langle f, \Psi^{(n+1)} \rangle_{n+1} \quad (2.83)$$

and the **creation operator** as $a^\dagger(f) := (a(f))^*$. These operators satisfy some basic properties, that we recall in the following Proposition.

Proposition 2.4.11. *Let $\{f_j\}_j$ be an orthonormal basis of \mathfrak{h} , then*

- *a and a^\dagger satisfy the **canonical commutation relations**, i.e. for any $f, g \in \mathfrak{h}$*

$$[a(f), a^\dagger(g)] = \langle f, g \rangle, \quad (2.84)$$

$$[a(f), a(g)] = [a^\dagger(f), a^\dagger(g)] = 0; \quad (2.85)$$

- *Let $f, g, h, k \in \mathfrak{h}$, then*

$$(a^\dagger(f) a(g) \Psi)^{(n)} = \sum_{r=1}^n |f\rangle \langle g|_r \Psi^{(n)}, \quad (2.86)$$

$$(a^\dagger(f) a^\dagger(g) a(h) a(k) \Psi)^{(n)} = \sum_{\substack{1 \leq r, s \leq n, \\ r \neq s}} |f\rangle \langle g|_j |h\rangle \langle k|_k \Psi^{(n)}. \quad (2.87)$$

*In particular, if the **number operator** \mathcal{N} is defined as $(\mathcal{N}\Psi)^{(n)} := n\Psi^{(n)}$, then*

$$\sum_j a^\dagger(f_j) a(f_j) = \mathcal{N}. \quad (2.88)$$

In [Case A](#) we can consider the set of eigenfunctions of h given by $\varphi_{\mathbf{p}}(\mathbf{x}) := |\Lambda|^{-\frac{1}{2}} e^{i\mathbf{p}\cdot\mathbf{x}}$, with $\mathbf{p} \in \Lambda^* := \left(\frac{2\pi}{L}\mathbb{Z}\right)^d$ and set $a_{\mathbf{p}} := a(\varphi_{\mathbf{p}})$ and $a_{\mathbf{p}}^\dagger := a^\dagger(\varphi_{\mathbf{p}})$. Then, in the N particle sector (i.e. the eigenspace identified by $\mathcal{N} = N$) we get

$$H_N := \mathbb{H}|_{\mathcal{H}_N} = \sum_{\mathbf{p} \in \Lambda^*} |\mathbf{p}|^2 a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \frac{1}{2\sqrt{|\Lambda|}} \sum_{\mathbf{p}, \mathbf{q}, \mathbf{r} \in \Lambda^*} \widehat{v}(\mathbf{r}) a_{\mathbf{p}+\mathbf{r}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{p}} a_{\mathbf{q}+\mathbf{r}} \quad (2.89)$$

where we recall that \widehat{v} stands for the **Fourier transform** of v , i.e.

$$\widehat{v}(\mathbf{r}) := \frac{1}{\sqrt{|\Lambda|}} \int_{\Lambda} d\mathbf{x} e^{-i\mathbf{p}\cdot\mathbf{x}} v(\mathbf{x}). \quad (2.90)$$

If we now assume that there is complete BEC, then the occupation number of the state φ_0 is of order N , i.e. $a_0^\dagger a_0 \approx N$. In [\[B47\]](#) Bogoliubov introduced what is nowadays called **Bogoliubov approximation** for the Hamiltonian \mathbb{H} , consisting of replacing a_0 and a_0^\dagger with \sqrt{N} and then dropping all terms higher than quadratic. We denote the resulting Hamiltonian as \mathbb{H}^{Bog} , i.e.

$$\mathbb{H}^{\text{Bog}} = \frac{N(N-1)}{2} \widehat{v}(0) + \sum_{\mathbf{p} \neq 0} |\mathbf{p}|^2 a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \quad (2.91)$$

$$+ \frac{N}{2\sqrt{|\Lambda|}} \sum_{\mathbf{p} \neq 0} \widehat{v}(\mathbf{p}) \left(a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + a_{-\mathbf{p}}^\dagger a_{-\mathbf{p}} + a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger + a_{\mathbf{p}} a_{-\mathbf{p}} \right) \quad (2.92)$$

$$= \frac{N(N-1)}{2} \widehat{v}(0) + \sum_{\mathbf{p} \neq 0} \left(|\mathbf{p}|^2 + \frac{N}{|\Lambda|} \widehat{v}(\mathbf{p}) \right) a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \quad (2.93)$$

$$+ \frac{N}{2\sqrt{|\Lambda|}} \sum_{\mathbf{p} \neq 0} \widehat{v}(\mathbf{p}) \left(a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger + a_{\mathbf{p}} a_{-\mathbf{p}} \right). \quad (2.94)$$

Now the key feature of \mathbb{H}^{Bog} is that it can be explicitly diagonalized, i.e., if we set

$$d_{\mathbf{p}} := \cosh \alpha_{\mathbf{p}} a_{\mathbf{p}} + \sinh \alpha_{\mathbf{p}} a_{\mathbf{p}}^\dagger, \quad (2.95)$$

$$d_{\mathbf{p}}^\dagger := \cosh \alpha_{\mathbf{p}} a_{\mathbf{p}}^\dagger + \sinh \alpha_{\mathbf{p}} a_{\mathbf{p}}, \quad (2.96)$$

$$\alpha_{\mathbf{p}} := \operatorname{arctanh} \left(\frac{|\mathbf{p}|^2 + \frac{N}{|\Lambda|} \widehat{v}(\mathbf{p}) - \sqrt{|\mathbf{p}|^2 \left(|\mathbf{p}|^2 + \frac{2N}{|\Lambda|} \widehat{v}(\mathbf{p}) \right)}}{\frac{N}{|\Lambda|} \widehat{v}(\mathbf{p})} \right), \quad (2.97)$$

$$e_{\mathbf{p}} := \sqrt{|\mathbf{p}|^2 \left(|\mathbf{p}|^2 + \frac{2N}{|\Lambda|} \widehat{v}(\mathbf{p}) \right)}, \quad (2.98)$$

$$E^{\text{Bog}} := -\frac{1}{2} \sum_{\mathbf{p} \neq 0} \left[|\mathbf{p}|^2 + \frac{N}{|\Lambda|} \widehat{v}(\mathbf{p}) - \sqrt{|\mathbf{p}|^2 \left(|\mathbf{p}|^2 + \frac{2N}{|\Lambda|} \widehat{v}(\mathbf{p}) \right)} \right], \quad (2.99)$$

then $d_{\mathbf{p}}$ and $d_{\mathbf{p}}^\dagger$ satisfy canonical commutation relations and we get

$$\mathbb{H}^{\text{Bog}} = \frac{N(N-1)}{2} \widehat{v}(\mathbf{0}) + E^{\text{Bog}} + \sum_{\mathbf{p} \neq 0} e_{\mathbf{p}} d_{\mathbf{p}}^\dagger d_{\mathbf{p}}. \quad (2.100)$$

The Bogoliubov theory is expected to provide a better approximation of the ground state of the many-body Hamiltonian if there is BEC.

The first rigorous results in this direction were proven by Grec and Seiringer in [S11; GS13] in the mean-field limit. In [Case A](#) the result reads as follows.

Theorem 2.4.12 (Seiringer, 2011). *Let E^{Bog} be defined as in (2.100). Then,*

$$E_N^{\text{mf}} = NE^{\text{H}} + E^{\text{Bog}} + \mathcal{O}\left(N^{-\frac{1}{2}}\right). \quad (2.101)$$

Moreover, the spectrum of $H_N^{\text{mf}} - E_N^{\text{mf}}$ below a threshold ξ is equal to finite sums of the form

$$\sum_{\mathbf{p} \neq 0} e_{\mathbf{p}} n_{\mathbf{p}} + \mathcal{O}\left(\xi^{\frac{3}{2}} N^{-\frac{1}{2}}\right). \quad (2.102)$$

The results describes well the spectrum of the Hamiltonian but tells nothing about the actual excited states; such information was derived by Lewin, Nam, Serfaty and Solovej in [LNSS15], exploiting a Fock space representation of the excitations over the ground state. This new idea was then used by Boccato, Brennecke, Cenatiempo and Schlein in [BBCS1], and more recently in [BBCS18], to investigate further the excitation spectrum of the Hamiltonian in the Gross-Pitaevskii regime.

Theorem 2.4.13 (Boccato, Brennecke, Cenatiempo, Schlein, 2018). *Let E_N^{GP} be defined as in (2.72). Set E and E^{Bog} as*

$$E := \frac{1}{2} \widehat{v}(0) + \frac{1}{2} \sum_{k=1}^{+\infty} \frac{(-1)^k}{(2N)^k} \times \sum_{\mathbf{p}_1, \dots, \mathbf{p}_k \in \Lambda^* \setminus \{0\}} \frac{\widehat{v}(\mathbf{p}_1/N)}{\mathbf{p}_1^2} \left(\prod_{j=1}^{k-1} \frac{\widehat{v}((\mathbf{p}_j - \mathbf{p}_{j-1})/N)}{\mathbf{p}_{j-1}^2} \right) \widehat{v}(\mathbf{p}_k/N), \quad (2.103)$$

$$E^{\text{Bog}} := -\frac{1}{2} \sum_{\mathbf{p} \neq 0} \left[|\mathbf{p}|^2 + 8\pi a - \sqrt{|\mathbf{p}|^4 + 16\pi a |\mathbf{p}|^2} - \frac{(8\pi a)^2}{2|\mathbf{p}|^2} \right], \quad (2.104)$$

then,

$$E_N^{\text{GP}} = NE + E^{\text{Bog}} + \mathcal{O}\left(N^{-\frac{1}{4}}\right). \quad (2.105)$$

Moreover, the spectrum of $H_N^{\text{GP}} - E_N^{\text{GP}}$ below a threshold ξ is equal to finite sums of the form

$$\sum_{\mathbf{p} \neq 0} n_{\mathbf{p}} \sqrt{|\mathbf{p}|^4 + 16\pi a |\mathbf{p}|^2} + \mathcal{O}\left(N^{-\frac{1}{4}} (1 + \xi^3)\right). \quad (2.106)$$

2.5 Thomas-Fermi Limit

We now introduce the setting we are going to study in the rest of the Thesis. We discussed before the Gross-Pitaevskii limit, which is a special dilute limit but not the only possible one. Another relevant dilute limit is the so-called **Thomas-Fermi (TF) limit**, which is named after the effective energy functional reminding the TF functional appearing in the theory of fermionic systems, and which importance in experiments was already mentioned in [1.3.2](#).

In the Gross-Pitaevskii limit we assumed that Na was constant as $N \rightarrow +\infty$. At the same time, to describe many experimental settings is useful to consider Na as a large parameter, and therefore a different description must be used. The TF limit consider a framework in which Na goes to infinity. We will now see how to implement it mathematically. We consider the following many-body Hamiltonian

$$H_N^{\text{TF}} := \sum_{j=1}^N h_j + \frac{g_N}{N} \sum_{1 \leq j < k \leq N} N^{3\beta} v \left(N^\beta (\mathbf{x}_j - \mathbf{x}_k) \right), \quad (2.107)$$

Where $\beta \in (0, 1)$ and $g_N \gg 1$. We analyze the scattering length of the potential in the following Proposition.

Proposition 2.5.1. *Let $v \in C_0^\infty(\mathbb{R}^3)$ be positive and radial and let a_N be the scattering length of $v_N(\mathbf{x}) := g_N N^{3\beta-1} v(N^\beta \mathbf{x})$. Assume that $g_N \ll N^{1-\beta}$, then*

$$a_N = \frac{g_N}{8\pi N} \int_{\mathbb{R}^3} d\mathbf{x} v(\mathbf{x}) + \mathcal{O}\left(\frac{g_N^2}{N^{2-\beta}}\right). \quad (2.108)$$

Proof. Recall that if f is the scattering solution and solves

$$-\Delta f + \frac{1}{2} v_N f = 0, \quad (2.109)$$

then the scattering length satisfies

$$a_N = \frac{1}{8\pi} \int_{\mathbb{R}^3} d\mathbf{x} v_N(\mathbf{x}) f(\mathbf{x}). \quad (2.110)$$

If we now set $h(\mathbf{y}) := f(N^{-\beta} \mathbf{y})$, h solves a similar equation:

$$-\Delta h + \frac{g_N N^{\beta-1}}{2} v h = 0. \quad (2.111)$$

The structure of the equation is now the same we found in Proposition [2.4.2](#) and, proceeding similarly, we get the result.

□

Given that g_N is a multiplicative constant in front of the potential we can assume that the integral of v is equal to 1. Let us now compute the energy of a completely factorized state $\Psi_T := \phi^{\otimes N}$ and show that the kinetic term is subleading with respect to the potential as $N \gg 1$. More explicitly, if we consider a trapping potential of the form⁷ $U(\mathbf{x}) = |\mathbf{x}|^s$, with $s \geq 2$, we get

$$\frac{1}{N} \langle H_N^{\text{TF}} \rangle_{\Psi_T} \approx \int_{\mathbb{R}^3} d\mathbf{x} \left\{ |\nabla \phi(\mathbf{x})|^2 + U(\mathbf{x}) |\phi(\mathbf{x})|^2 + \frac{g_N}{2} |\phi(\mathbf{x})|^4 \right\} \quad (2.112)$$

$$=: \mathcal{E}_{g_N}^{\text{GP}}[\phi]. \quad (2.113)$$

If we then set

$$E_{g_N}^{\text{GP}} := \inf \{ \mathcal{E}_{g_N}^{\text{GP}}[\phi] : \phi \in L^2(\mathbb{R}^3) \}, \quad (2.114)$$

$$\mathcal{E}_r^{\text{GP}}[\phi] := \int_{\mathbb{R}^3} d\mathbf{x} \left\{ g_N^{-\frac{s+2}{s+3}} |\nabla \phi(\mathbf{x})|^2 + U(\mathbf{x}) |\phi(\mathbf{x})|^2 + \frac{1}{2} |\phi(\mathbf{x})|^4 \right\}, \quad (2.115)$$

$$E_r^{\text{GP}} := \inf \{ \mathcal{E}_r^{\text{GP}}[\phi] : \phi \in L^2(\mathbb{R}^3) \}, \quad (2.116)$$

then $E_{g_N}^{\text{GP}}$ satisfies the interesting scaling property

$$E_{g_N}^{\text{GP}} = g_N^{\frac{s}{s+3}} E_r^{\text{GP}}, \quad (2.117)$$

and the kinetic term is depleted by the small term in front of it.

In [LSY00] Lieb, Seiringer and Yngvason were able to prove that the first order of the energy is reproduced by a simple minimization problem for the density, defined as

$$\mathcal{F}_g[\rho] := \int_{\mathbb{R}^3} d\mathbf{x} \left\{ U(\mathbf{x}) \rho(\mathbf{x}) + \frac{g}{2} \rho^2(\mathbf{x}) \right\} \quad (2.118)$$

$$F_g := \inf \{ \mathcal{F}_g[\rho] : \rho \geq 0, \|\rho\|_1 = 1 \} \\ = \mathcal{F}[\rho_g]. \quad (2.119)$$

Under the above assumptions on U , one can prove the scaling property $F_g = g^{\frac{s}{s+3}} F_1$ and $\rho_g(\mathbf{x}) = g^{-\frac{3}{s+3}} \rho_1(g^{-\frac{1}{s+3}} \mathbf{x})$.

Proposition 2.5.2. *If $g_N \ll N^{\frac{2(s+3)}{3(s+2)}}$, then the gas is dilute in the Thomas-Fermi limit.*

Proof. A simple calculation shows that $\bar{\rho}_{g_N} \approx N g_N^{-\frac{3}{s+3}}$. From Proposition 2.5.1 we get that $a_N \approx N^{-1} g_N$. Therefore $a_N \bar{\rho}_{g_N}^{\frac{1}{3}} \approx N^{-\frac{2}{3}} g_N^{\frac{s+2}{s+3}} \ll 1$.

□

⁷We choose here a homogeneous potential so that the computations are easier. One can deal in a similar way with non-homogeneous potentials, provided that U is asymptotically homogeneous, i.e. $\frac{V(\mathbf{x})}{|\mathbf{x}|^s} \rightarrow C > 0$ as $|\mathbf{x}| \rightarrow +\infty$.

Defining then $E_N^{\text{TF}} := \inf \sigma(H_N^{\text{TF}})$ and the density of the system ρ^{TF} as

$$\rho^{\text{TF}}(\mathbf{x}) := \int_{\mathbb{R}^3} d\mathbf{x}_2 \dots d\mathbf{x}_N |\Psi^{\text{TF}}(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N)|^2, \quad (2.120)$$

the following result holds true.

Theorem 2.5.3 (Lieb, Seiringer, Yngvason, 2001). *Let $U(\mathbf{x}) = |\mathbf{x}|^s$ and $v \in C_0^\infty(\mathbb{R}^3)$, then*

$$\begin{aligned} E_N^{\text{TF}} &= NF_{g_N}(1 + o(1)) \\ &= Ng_N^{\frac{s}{s+3}} F_1(1 + o(1)), \end{aligned} \quad (2.121)$$

$$g_N^{\frac{3}{s+3}} \rho^{\text{TF}}\left(g_N^{\frac{1}{s+3}} \mathbf{x}\right) \xrightarrow{w-L^1(\mathbb{R}^3)} \rho_1(\mathbf{x}) \quad (2.122)$$

Even if there is convergence of the densities, this is not enough to ensure convergence of the 1-reduced density matrix. However, we will prove full BEC in Chapter 3.

As far as our knowledge goes, there is no proof that condensation is preserved as time evolves. In Chapter 4 we will discuss precisely this question. Indeed, assuming condensation in the initial state, one can use techniques similar to [P11] to get that condensation is preserved also at later times.

CHAPTER 3

Ground State Energy and BEC in the TF Regime

In this Chapter, we discuss BEC in the TF regime. Furthermore, we investigate the next-to-leading order approximation for the ground state energy of the system via the Bogoliubov approximation. Based on a joint work in progress with Michele Correggi.

We consider N particles confined in a box of side length L in d dimensions $\Lambda := [-\frac{L}{2}, \frac{L}{2}]^d$. The many-body Hamiltonian in this framework is given by

$$H_N := - \sum_{j=1}^N \Delta_j + \frac{g_N}{N-1} \sum_{1 \leq j < k \leq N} v_N(x_j - x_k) \quad (3.1)$$

acting on $\mathcal{H}_N := \mathfrak{h}^{\otimes_s N}$ where $\mathfrak{h} := L_{\text{per}}^2(\Lambda)$ with periodic boundary conditions. We assume that $g_N \rightarrow +\infty$ and we will make the following assumptions on v_N .

We recall that for any $\varphi \in \mathfrak{h}$ its Fourier transform $\widehat{\varphi}$ is defined as

$$\widehat{\varphi}(\mathbf{p}) := \frac{1}{L^{\frac{d}{2}}} \int_{\Lambda} d\mathbf{x} \, e^{-i\mathbf{p} \cdot \mathbf{x}} \varphi(\mathbf{x}), \quad \mathbf{p} \in \Lambda^* := \left(\frac{2\pi}{L} \mathbb{Z} \right)^d.$$

Assumption 3.0.1. *Let $v_N(\mathbf{x}) := N^{d\beta} v(N^\beta \mathbf{x})$, with $\beta \in (0, 1)$ and $v \in C_0^\infty(\Lambda)$. We also assume that v is of **positive type**, i.e. $\widehat{v} \geq 0$.*

Our main goal in this Chapter is to prove that there is BEC in the ground state of the system, i.e. as $N \rightarrow +\infty$, a macroscopic fraction of the particles occupies the one-particle ground state, i.e. the constant wave function.

3.1 Ground State Energy and BEC

We first define what a ground state is.

Definition 3.1.1. Let $E_0(N)$ be the **ground state energy** of H_N , i.e.

$$E_0(N) := \inf \sigma(H_N) \quad (3.2)$$

$$= \inf \{ \langle \Psi, H_N \Psi \rangle \mid \Psi \in \mathcal{H}_N, \|\Psi\| = 1 \}. \quad (3.3)$$

We denote by Ψ_0 the unique (up to an overall phase) **ground state** of H_N , i.e. the minimizer of (3.3), which satisfies the Schrödinger equation $H_N \Psi_0 = E_0(N) \Psi_0$, at least in weak sense.

We want to prove the following Theorem.

Theorem 3.1.2. Let v be as in Assumption 3.0.1. Then,

$$E_0(N) = \frac{N}{2L^{\frac{d}{2}}} g_N \widehat{v}(\mathbf{0}) + \mathcal{O}(g_N N^{d\beta}). \quad (3.4)$$

Furthermore, there is also BEC in the one-particle ground state. This is the content of next Theorem.

Theorem 3.1.3. Let v be as in Assumption 3.0.1. Let also Ψ_0 be the ground state of H_N as in Definition 3.1.1. Then, if $\xi_0 := L^{-\frac{d}{2}}$ we get

$$\left\| \gamma_{\Psi_0}^{(1)} - P_{\xi_0} \right\|_1 \leq C \sqrt{L^2 N^{d\beta-1} g_N} \left(1 + \sqrt{L^2 N^{d\beta-1} g_N} \right) \quad (3.5)$$

where $\gamma_{\Psi_0}^{(1)}$ is the 1-reduced density matrix of the many-body state Ψ_0 . In particular, if $\beta < \frac{1}{d}$ and $g_N \ll N^{1-d\beta}$, there is BEC for any fixed $L \geq 0$.

In the following we set $P := P_{\xi_0}$ and $Q := 1 - P$ for short. Furthermore, P_j and Q_j will denote copies of the operators P and Q acting on the j -th particle Hilbert space \mathfrak{h} . The final goal is to estimate the fraction of the number of particles outside of the condensate. To do so, we define $\mathcal{N}^>$ as the **number of particles not in the constant wave function** (or number of excited particles), i.e., mathematically,

$$\mathcal{N}^> := \sum_{j=1}^N Q_j. \quad (3.6)$$

Given that ξ_0 is an eigenstate of the Laplacian, we easily see that $[-\Delta, P] = [-\Delta, Q] = 0$. Moreover, one has the lower bound $-\Delta \geq \left(\frac{2\pi}{L}\right)^2 Q$. Therefore, if we denote by T the **kinetic energy**, i.e.

$$T := \sum_{j=1}^N (-\Delta_j), \quad (3.7)$$

we get that

$$T \geq \left(\frac{2\pi}{L} \right)^2 \mathcal{N}^>. \quad (3.8)$$

To get a control on the number of excited particles, it is thus sufficient to bound T from above.

Now both results can actually be obtained as consequences of the next Proposition, which follows a key idea in [S11].

Proposition 3.1.4. *Let Ψ_0 and $E_0(N)$ be as in Definition 3.1.1. Then, for any v as in Assumption 3.0.1, the following bound holds*

$$-\frac{g_N N}{2(N-1)} \left(N^{d\beta} v(\mathbf{0}) - L^{-\frac{d}{2}} \widehat{v}(\mathbf{0}) \right) \leq E_0(N) - \frac{N}{2L^{\frac{d}{2}}} g_N \widehat{v}(\mathbf{0}) \leq 0. \quad (3.9)$$

Furthermore, if $\overline{\Psi}$ satisfies $\langle \overline{\Psi}, H_N \overline{\Psi} \rangle \leq E_N(\mathbf{0}) + \mu$ for some μ , then

$$\left(\frac{2\pi}{L} \right)^2 \langle \overline{\Psi}, N^> \overline{\Psi} \rangle \leq \langle \overline{\Psi}, T \overline{\Psi} \rangle \leq \frac{g_N N}{2(N-1)} \left(N^{d\beta} v(\mathbf{0}) - L^{-\frac{d}{2}} \widehat{v}(\mathbf{0}) \right) + \mu. \quad (3.10)$$

Proof. We consider the energy of the constant function, which yields the following upper bound to the many-body energy

$$E_0(N) \leq \langle \xi_0, H_N \xi_0 \rangle = \frac{N g_N}{2L^{\frac{d}{2}}} \widehat{v}_N(\mathbf{0}) = \frac{N g_N}{2L^{\frac{d}{2}}} \widehat{v}(\mathbf{0}). \quad (3.11)$$

To prove the lower bound, we first recall the Parseval identity, which for v reads

$$v(\mathbf{x}) = L^{-\frac{d}{2}} \sum_{\mathbf{p} \in \Lambda^*} \widehat{v}(\mathbf{p}) e^{i\mathbf{p} \cdot \mathbf{x}}. \quad (3.12)$$

Therefore we can rewrite the potential term in H_N as

$$\sum_{1 \leq j < k \leq N} v_N(\mathbf{x}_j - \mathbf{x}_k) = \frac{1}{2L^{\frac{d}{2}}} \sum_{1 \leq j, k \leq N} \sum_{\mathbf{p} \in \Lambda^*} \widehat{v}_N(\mathbf{p}) e^{i\mathbf{p} \cdot (\mathbf{x}_j - \mathbf{x}_k)} - \frac{N}{2} v_N(\mathbf{0}) \quad (3.13)$$

$$= \frac{1}{2L^{\frac{d}{2}}} \sum_{\mathbf{p} \in \Lambda^*} \widehat{v}_N(\mathbf{p}) \left| \sum_{j=1}^N e^{i\mathbf{p} \cdot \mathbf{x}_j} \right|^2 - \frac{N}{2} v_N(\mathbf{0}) \geq \frac{N^2}{2L^{\frac{d}{2}}} \widehat{v}(\mathbf{0}) - \frac{N}{2} v_N(\mathbf{0}), \quad (3.14)$$

where in the last inequality we used that $\widehat{v} \geq 0$.

From this lower bound, we deduce easily that, for any state $\Psi \in \mathcal{H}_N$, we have

$$\langle \Psi, H_N \Psi \rangle \geq \langle \Psi, T \Psi \rangle + \frac{g_N}{N-1} \left(\frac{N^2}{2L^{\frac{d}{2}}} \widehat{v}(\mathbf{0}) - \frac{N}{2} v_N(\mathbf{0}) \right) \quad (3.15)$$

$$\Rightarrow \langle \Psi, H_N \Psi \rangle - \frac{N}{2L^{\frac{d}{2}}} g_N \widehat{v}(\mathbf{0}) \geq \langle \Psi, T \Psi \rangle - \frac{g_N N}{2(N-1)} \left(v_N(\mathbf{0}) - L^{-\frac{d}{2}} \widehat{v}(\mathbf{0}) \right) \quad (3.16)$$

$$\geq -\frac{g_N N}{2(N-1)} \left(v_N(\mathbf{0}) - L^{-\frac{d}{2}} \widehat{v}(\mathbf{0}) \right), \quad (3.17)$$

which gives us the lower bound in (3.9).

Moreover, suppose that $\bar{\Psi}$ satisfies the hypotheses of the Proposition, then, the lower bound we have just proven implies that

$$\langle \bar{\Psi}, T \bar{\Psi} \rangle \leq E_0(N) + \mu - \frac{g_N}{N-1} \left(\frac{N^2}{2L^{\frac{d}{2}}} \widehat{v}(\mathbf{0}) - \frac{N}{2} v_N(\mathbf{0}) \right) \quad (3.18)$$

$$\leq \frac{g_N N}{2(N-1)} \left(v_N(\mathbf{0}) - L^{-\frac{d}{2}} \widehat{v}(\mathbf{0}) \right) + \mu, \quad (3.19)$$

and the final bound follows from $-\Delta \geq \left(\frac{2\pi}{L}\right)^2 Q$ and the definition of v_N .

□

Proof (Theorem 3.1.2 and 3.1.3). Theorem 3.1.2 follows from Proposition 3.1.4. As a first step to prove Theorem 3.1.3, we apply Proposition 3.1.4 to the ground state energy to get that, for a suitable constant C independent of N and L ,

$$\langle \Psi_0, N^> \Psi_0 \rangle \leq CL^2 N^{d\beta} g_N. \quad (3.20)$$

Now, for a generic state ψ and a bounded operator A , we have

$$\langle \Psi, A \Psi \rangle = \langle \Psi, Q_1 A Q_1 \Psi \rangle + \langle \Psi, P_1 A Q_1 \Psi \rangle \quad (3.21)$$

$$+ \langle \Psi, Q_1 A P_1 \Psi \rangle + \langle \xi_0, A \xi_0 \rangle \langle \Psi, P_1 \Psi \rangle. \quad (3.22)$$

Therefore, we get that

$$\left\| \gamma_{\Psi_0}^{(1)} - P \right\|_1 = \sup_{\|A\|=1} \left| \text{tr} \left\{ A \left(\gamma_{\Psi_0}^{(1)} - P \right) \right\} \right| \quad (3.23)$$

$$= \sup_{\|A\|=1} |\langle \Psi_0, A_1 \Psi_0 \rangle - \langle \xi_0, A \xi_0 \rangle| \quad (3.24)$$

$$= \sup_{\|A\|=1} |\langle \Psi_0, P_1 A_1 Q_1 \Psi_0 \rangle + \langle \Psi_0, Q_1 A_1 P_1 \Psi_0 \rangle| \quad (3.25)$$

$$+ \langle \Psi_0, Q_1 A_1 Q_1 \Psi_0 \rangle - \langle \xi_0, A \xi_0 \rangle \langle \Psi_0, Q_1 \Psi_0 \rangle| \quad (3.26)$$

$$\leq 2 \|Q_1 \Psi_0\| (1 + \|Q_1 \Psi_0\|). \quad (3.27)$$

The definition of $N^>$ and the symmetry of Ψ_0 implies that $\|Q_1\Psi_0\|^2 = N^{-1}\langle\Psi_0, N^>\Psi_0\rangle$ and therefore

$$\left\|\gamma_{\Psi_0}^{(1)} - P\right\|_1 \leq \frac{2}{\sqrt{N}} \sqrt{\langle\Psi_0, N^>\Psi_0\rangle} \left(1 + \frac{1}{\sqrt{N}} \sqrt{\langle\Psi_0, N^>\Psi_0\rangle}\right) \quad (3.28)$$

$$\leq C \sqrt{L^2 N^{d\beta-1} g_N} \left(1 + \sqrt{L^2 N^{d\beta-1} g_N}\right). \quad (3.29)$$

□

3.2 The Bogoliubov Theory

To investigate the next order approximation of the energy, it is useful to think in terms of excitations with respect to the ground state, which in turn are easier understood exploiting the formalism of Fock spaces. We recall here some of the key properties of such spaces.

3.2.1 Fock Space

We now recall and expand some of the definitions already introduced in Section 2.4.4. In our case, the Fock space \mathcal{F} reads

$$\mathcal{F} := \bigoplus_{k \geq 0} L^2(\Lambda)^{\otimes_{\text{s}} k}, \quad (3.30)$$

which is conveniently used to describe a system where the number of particles is not fixed, i.e. particles can be destroyed or created. Let $\varphi \in L^2(\Lambda)$ be a one-particle state; for any $\Psi = (\Psi^{(k)})_{k \geq 0} \in \mathcal{F}$ we define the **annihilation operator** $a(\varphi)$ (respectively the **creation operator** $a^\dagger(\varphi)$) as

$$(a(\varphi)\Psi)^{(k)} := \sqrt{k+1} \int_{\Lambda} d\mathbf{x} \, \overline{\varphi(\mathbf{x})} \Psi^{(k+1)}(\mathbf{x}, \mathbf{x}_1, \dots, \mathbf{x}_k); \quad (3.31)$$

$$(a^\dagger(\varphi)\Psi)^{(k)} := \frac{1}{\sqrt{k}} \sum_{j=1}^k \varphi(\mathbf{x}_j) \Psi^{(k-1)}(\mathbf{x}_1, \dots, \mathbf{x}_{j-1}, \mathbf{x}_{j+1}, \dots, \mathbf{x}_k). \quad (3.32)$$

Notice that with such definitions we have $a(\varphi)^* = a^\dagger(\varphi)$ for any $\varphi \in L^2(\Lambda)$, and a and a^\dagger satisfy the **canonical commutation relations (CCR)**:

$$\left[a(\varphi), a^\dagger(\psi)\right] = \langle\varphi, \psi\rangle, \quad \left[a(\varphi), a(\psi)\right] = \left[a^\dagger(\varphi), a^\dagger(\psi)\right] = 0. \quad (3.33)$$

Since we are interested in condensation on the constant function ξ_0 , it is convenient to consider excitations generated by creation or annihilation operators on specific states forming with ξ_0 a complete orthonormal system. In particular, given that the kinetic term controls the number operator, we are going to use the eigenfunctions of the Laplace operator $-\Delta$ with periodic boundary conditions. Let then $\xi_{\mathbf{p}}(\mathbf{x}) := \frac{1}{L^{\frac{d}{2}}} e^{-i\mathbf{p}\cdot\mathbf{x}}$, with $\mathbf{p} \in \Lambda^*$. Then, we set $a_{\mathbf{p}} := a(\xi_{\mathbf{p}})$ and $a_{\mathbf{p}}^\dagger := a^\dagger(\xi_{\mathbf{p}})$ for short. The CCRs thus become

$$[a_{\mathbf{p}}, a_{\mathbf{q}}^\dagger] = \delta_{\mathbf{p}, \mathbf{q}}, \quad [a_{\mathbf{p}}, a_{\mathbf{q}}] = [a_{\mathbf{p}}^\dagger, a_{\mathbf{q}}^\dagger] = 0, \quad \forall \mathbf{p}, \mathbf{q} \in \Lambda^*. \quad (3.34)$$

These operators satisfy some interesting properties. For instance, if we define the **number operator** \mathcal{N} as $(\mathcal{N}\Psi)^{(k)} := n\Psi^{(k)}$, then we get

$$\sum_{\mathbf{p} \in \Lambda^*} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} = \mathcal{N}, \quad (3.35)$$

which in particular implies that $\mathcal{N}a_{\mathbf{p}} = a_{\mathbf{p}}(\mathcal{N} - 1)$ and $\mathcal{N}a_{\mathbf{p}}^\dagger = a_{\mathbf{p}}^\dagger(\mathcal{N} + 1)$, as intuitively guessed by the particle counting analogy.

The different sectors of the Fock space \mathcal{F} are then identified by the number of particles. The action of $a_{\mathbf{p}}^\dagger a_{\mathbf{q}}$ in the sector with n particles is explicit and given by

$$a_{\mathbf{p}}^\dagger a_{\mathbf{q}} = \sum_{j=1}^n |\xi_{\mathbf{p}}\rangle \langle \xi_{\mathbf{q}}|_j, \quad a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{r}} a_{\mathbf{s}} = \sum_{1 \leq j \neq k \leq n} |\xi_{\mathbf{p}}\rangle \langle \xi_{\mathbf{r}}|_j |\xi_{\mathbf{q}}\rangle \langle \xi_{\mathbf{s}}|_k. \quad (3.36)$$

The idea is now to represent the Hamiltonian in (3.1) as an operator acting only on the N -th sector of the Fock space and rewrite it in terms of creation and annihilation operators. The kinetic term is easily given by $T = \sum_{\mathbf{p} \in \Lambda^*} |\mathbf{p}|^2 a_{\mathbf{p}}^\dagger a_{\mathbf{p}}$, while the interaction becomes

$$\sum_{j < k} v_N(\mathbf{x}_j - \mathbf{x}_k) = \frac{1}{2L^{\frac{d}{2}}} \sum_{j \neq k} \sum_{\mathbf{r} \in \Lambda^*} \widehat{v}_N(\mathbf{r}) e^{i\mathbf{r} \cdot (\mathbf{x}_j - \mathbf{x}_k)} \quad (3.37)$$

$$= \frac{1}{2L^{\frac{d}{2}}} \sum_{\mathbf{p}, \mathbf{q}, \mathbf{r} \in \Lambda^*} \widehat{v}_N(\mathbf{r}) \sum_{j \neq k} |\xi_{\mathbf{p}+\mathbf{r}}\rangle \langle \xi_{\mathbf{p}}|_j |\xi_{\mathbf{q}}\rangle \langle \xi_{\mathbf{q}+\mathbf{r}}|_k \quad (3.38)$$

$$= \frac{1}{2L^{\frac{d}{2}}} \sum_{\mathbf{p}, \mathbf{q}, \mathbf{r} \in \Lambda^*} \widehat{v}_N(\mathbf{r}) a_{\mathbf{p}+\mathbf{r}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{p}} a_{\mathbf{q}+\mathbf{r}}. \quad (3.39)$$

Hence the Hamiltonian H_N acting on the Fock space \mathcal{F} reads¹

$$H_N = \sum_{\mathbf{p} \in \Lambda^*} |\mathbf{p}|^2 a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \frac{gN}{2NL^{\frac{d}{2}}} \sum_{\mathbf{p}, \mathbf{q}, \mathbf{r} \in \Lambda^*} \widehat{v}\left(\frac{\mathbf{r}}{N^\beta}\right) a_{\mathbf{p}+\mathbf{r}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{p}} a_{\mathbf{q}+\mathbf{r}}, \quad (3.40)$$

¹Notice that now N is a parameter, which equals the number of particles only in the N -th sector.

and coincides on the sector with N particles with the Hamiltonian defined in (3.1). More in general, given that $[\mathcal{N}, H_N] = 0$, H_N maps the n -th sector to itself, i.e. H_N is block diagonal with respect to the particle sector decomposition of \mathcal{F} . This will be useful later.

3.2.2 Towards the First Order Correction

We now investigate the Fock space structure of excitations. We recall the definition of the symmetric product of two different states: let $\varphi_k \in \mathfrak{h}^{\otimes_s k}$, with $k \in \{k_1, k_2\}$. Then $\varphi_{k_1} \otimes_s \varphi_{k_2} \in \mathfrak{h}^{\otimes_s(k_1+k_2)}$, where²

$$\begin{aligned} (\varphi_{k_1} \otimes_s \varphi_{k_2})(\mathbf{x}_1, \dots, \mathbf{x}_{k_1+k_2}) &:= \\ &= \frac{1}{\sqrt{k_1!k_2!(k_1+k_2)!}} \sum_{\sigma \in S_{k_1+k_2}} \varphi_{k_1}(\mathbf{x}_{\sigma(1)}, \dots, \mathbf{x}_{\sigma(k_1)}) \times \\ &\quad \times \varphi_{k_2}(\mathbf{x}_{\sigma(k_1+1)}, \dots, \mathbf{x}_{\sigma(k_1+k_2)}). \end{aligned} \quad (3.41)$$

We now consider the excitations with respect to the condensate in the constant function ξ_0 and set $\mathfrak{h}_+ := \{\xi_0\}^\perp$; then, there are uniquely defined functions $\Psi_k \in \mathfrak{h}_+^{\otimes_s k}$, such that

$$\Psi = \Psi_0 \xi_0^{\otimes N} + \Psi_1 \otimes_s \xi_0^{\otimes(N-1)} + \Psi_2 \otimes_s \xi_0^{\otimes(N-2)} + \dots + \Psi_N. \quad (3.42)$$

If one then defines $\mathcal{F}_+ := \bigoplus_{k \geq 0} \mathfrak{h}_+^{\otimes_s k}$, the **excitation Fock space** is the subspace

$$\mathcal{F}_+^{\leq N} := \bigoplus_{k=0}^N \mathfrak{h}_+^{\otimes_s k}. \quad (3.43)$$

Furthermore, the map $U : \Psi \mapsto \{\Psi_k\}_{k=0}^N$ is **unitary** from \mathcal{H}_N to $\mathcal{F}_+^{\leq N}$, and

$$(U_N \Psi)_k = [1 - |\xi_0\rangle\langle\xi_0|]^{\otimes k} \frac{a_0^{N-k}}{\sqrt{(N-k)!}} \Psi, \quad (3.44)$$

$$U_N^* \left(\{\Psi_k\}_{k=0}^N \right) = \sum_{k=0}^N \frac{a_0^{\dagger N-k}}{\sqrt{(N-k)!}} \Psi_k. \quad (3.45)$$

Since we are interested in the spectral properties of H_N we aim at computing $U_N H_N U_N^* =: \mathcal{L}_N$. The number operator in the Fock space here represents the number of excitations and we denote it by \mathcal{N}_+ ; note that $0 \leq \mathcal{N}_+ \leq N$. We

²We recall that S_k is the group of the permutations of k indistinguishable elements.

also denote the non-zero momenta as $\Lambda_+^* := \Lambda^* \setminus \{\mathbf{0}\}$, so that $\sum_{\mathbf{p} \in \Lambda_+^*} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} = \mathcal{N}_+$. It is also convenient to introduce new creation and annihilation operators $b_{\mathbf{p}}$ and $b_{\mathbf{p}}^\dagger$ as

$$b_{\mathbf{p}} := \sqrt{\frac{N - \mathcal{N}_+}{N}} a_{\mathbf{p}}, \quad b_{\mathbf{p}}^\dagger := a_{\mathbf{p}}^\dagger \sqrt{\frac{N - \mathcal{N}_+}{N}}. \quad (3.46)$$

Indeed, with this definitions, we get

$$U_N \left(a_{\mathbf{0}}^\dagger a_{\mathbf{0}} \right) U_N^* = N - \mathcal{N}_+, \quad (3.47)$$

$$U_N \left(a_{\mathbf{0}}^\dagger a_{\mathbf{p}} \right) U_N^* = \sqrt{N} b_{\mathbf{p}}, \quad \mathbf{p} \in \Lambda_+^*, \quad (3.48)$$

$$U_N \left(a_{\mathbf{p}}^\dagger a_{\mathbf{0}} \right) U_N^* = \sqrt{N} b_{\mathbf{p}}^\dagger, \quad \mathbf{p} \in \Lambda_+^*, \quad (3.49)$$

$$U_N \left(a_{\mathbf{p}}^\dagger a_{\mathbf{q}} \right) U_N^* = a_{\mathbf{p}}^\dagger a_{\mathbf{q}}, \quad \mathbf{p}, \mathbf{q} \in \Lambda_+^*. \quad (3.50)$$

Notice that the b 's and b^\dagger 's do not satisfy the CCRs

$$[b_{\mathbf{p}}, b_{\mathbf{q}}] = [b_{\mathbf{p}}^\dagger, b_{\mathbf{q}}^\dagger] = 0, \quad [b_{\mathbf{p}}, b_{\mathbf{q}}^\dagger] = \delta_{\mathbf{p}, \mathbf{q}} \frac{N - \mathcal{N}_+}{N} - \frac{1}{N} a_{\mathbf{q}}^\dagger a_{\mathbf{p}}. \quad (3.51)$$

We are now able to write down \mathcal{L}_N in a more suitable way, as the sum of four different terms: $\mathcal{L}_N = \mathcal{L}_0 + \mathcal{L}_2 + \mathcal{L}_3 + \mathcal{L}_4$, where the label j stands for the degree of the polynomials in the creation and annihilation operators of the corresponding terms:

$$\mathcal{L}_0 := \frac{gN}{2NL^{\frac{d}{2}}} \widehat{v}(\mathbf{0}) (N - \mathcal{N}_+) (N + \mathcal{N}_+ - 1), \quad (3.52)$$

$$\begin{aligned} \mathcal{L}_2 := \sum_{\mathbf{p} \in \Lambda_+^*} |\mathbf{p}|^2 a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \frac{gN}{L^{\frac{d}{2}}} \sum_{\mathbf{p} \in \Lambda_+^*} \widehat{v}\left(\frac{\mathbf{p}}{N^\beta}\right) \left(b_{\mathbf{p}}^\dagger b_{\mathbf{p}} - \frac{1}{N} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \right) \\ + \frac{gN}{2L^{\frac{d}{2}}} \sum_{\mathbf{p} \in \Lambda_+^*} \widehat{v}\left(\frac{\mathbf{p}}{N^\beta}\right) \left(b_{\mathbf{p}} b_{-\mathbf{p}} + b_{\mathbf{p}}^\dagger b_{-\mathbf{p}}^\dagger \right), \end{aligned} \quad (3.53)$$

$$\mathcal{L}_3 := \frac{gN}{\sqrt{N}L^{\frac{d}{2}}} \sum_{\substack{\mathbf{p}, \mathbf{q} \in \Lambda_+^*, \\ \mathbf{p} + \mathbf{q} \neq \mathbf{0}}} \widehat{v}\left(\frac{\mathbf{p}}{N^\beta}\right) \left(a_{\mathbf{p}}^\dagger a_{-\mathbf{q}} b_{\mathbf{p} + \mathbf{q}} + a_{-\mathbf{q}}^\dagger a_{\mathbf{p}} b_{\mathbf{p} + \mathbf{q}}^\dagger \right), \quad (3.54)$$

$$\mathcal{L}_4 := \frac{gN}{2NL^{\frac{d}{2}}} \sum_{\substack{\mathbf{p}, \mathbf{q} \in \Lambda_+^*, \mathbf{r} \in \Lambda^*, \\ \mathbf{p} + \mathbf{r} \neq \mathbf{0} \neq \mathbf{q} + \mathbf{r}}} \widehat{v}\left(\frac{\mathbf{r}}{N^\beta}\right) a_{\mathbf{p} + \mathbf{r}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{p}} a_{\mathbf{q} + \mathbf{r}}. \quad (3.55)$$

The intuition about the above decomposition is that, as heuristically suggested by Theorem 3.1.3, the operator \mathcal{N}_+ is small for large N . Moreover,

the operators $a_{\mathbf{p}}$ and $b_{\mathbf{p}}$ should be thought as controlled by $\sqrt{\mathcal{N}_+}$; hence the main part of the Hamiltonian \mathcal{H}_N is given by \mathbb{H}_N , i.e.

$$\mathbb{H}_N := \frac{g_N (N-1)}{2L^{\frac{d}{2}}} \widehat{v}(\mathbf{0}) + \sum_{\mathbf{p} \in \Lambda_+^*} \left[|\mathbf{p}|^2 b_{\mathbf{p}}^\dagger b_{\mathbf{p}} \right. \quad (3.56)$$

$$\left. + \frac{g_N}{2L^{\frac{d}{2}}} \widehat{v}\left(\frac{\mathbf{p}}{N^\beta}\right) \left(2b_{\mathbf{p}}^\dagger b_{\mathbf{p}} + b_{\mathbf{p}} b_{-\mathbf{p}} + b_{\mathbf{p}}^\dagger b_{-\mathbf{p}}^\dagger \right) \right] \quad (3.57)$$

$$= \frac{g_N (N-1)}{2L^{\frac{d}{2}}} \widehat{v}(\mathbf{0}) + \sum_{\mathbf{p} \in \Lambda_+^*} \left[\left(|\mathbf{p}|^2 + \frac{g_N}{L^{\frac{d}{2}}} \widehat{v}\left(\frac{\mathbf{p}}{N^\beta}\right) \right) b_{\mathbf{p}}^\dagger b_{\mathbf{p}} \right. \quad (3.58)$$

$$\left. + \frac{g_N}{2L^{\frac{d}{2}}} \widehat{v}\left(\frac{\mathbf{p}}{N^\beta}\right) \left(b_{\mathbf{p}} b_{-\mathbf{p}} + b_{\mathbf{p}}^\dagger b_{-\mathbf{p}}^\dagger \right) \right], \quad (3.59)$$

where $D_{\mathbf{p}} := |\mathbf{p}|^2$ and $V_{\mathbf{p}} := g_N L^{-\frac{d}{2}} \widehat{v}\left(\frac{\mathbf{p}}{N^\beta}\right)$.

From now on, we set $L = 1$. Equivalently, we can rescale all lengths by L and replace $g_N \rightarrow L^{-\frac{d}{2}} g_N$. Now, \mathbb{H}_N is a self-adjoint operator which is quadratic in b and b^\dagger . This implies that it is diagonalizable: let $0 \leq \alpha_{\mathbf{p}} < 1$ be a sequence with $\alpha_{-\mathbf{p}} = \alpha_{\mathbf{p}}$ and set

$$f_{\mathbf{p}} := \frac{b_{\mathbf{p}} + \alpha_{\mathbf{p}} b_{-\mathbf{p}}^\dagger}{\sqrt{1 - \alpha_{\mathbf{p}}^2}}, \quad f_{\mathbf{p}}^\dagger := \frac{b_{\mathbf{p}}^\dagger + \alpha_{\mathbf{p}} b_{-\mathbf{p}}}{\sqrt{1 - \alpha_{\mathbf{p}}^2}}. \quad (3.60)$$

Then, if we denote by $\epsilon_{\mathbf{p}}$ the energy associated to the momentum \mathbf{p} , we get

$$\begin{aligned} \sum_{\mathbf{p} \in \Lambda_+^*} \epsilon_{\mathbf{p}} f_{\mathbf{p}}^\dagger f_{\mathbf{p}} &= \sum_{\mathbf{p} \in \Lambda_+^*} \frac{\epsilon_{\mathbf{p}}}{1 - \alpha_{\mathbf{p}}^2} \left[(1 + \alpha_{\mathbf{p}}^2) b_{\mathbf{p}}^\dagger b_{\mathbf{p}} + \alpha_{\mathbf{p}} \left(b_{\mathbf{p}} b_{-\mathbf{p}} + b_{\mathbf{p}}^\dagger b_{-\mathbf{p}}^\dagger \right) \right] \\ &+ \left(\sum_{\mathbf{p} \in \Lambda_+^*} \frac{\epsilon_{\mathbf{p}} \alpha_{\mathbf{p}}^2}{1 - \alpha_{\mathbf{p}}^2} \right) \frac{N - \mathcal{N}_+}{N} - \frac{1}{N} \left(\sum_{\mathbf{p} \in \Lambda_+^*} \frac{\epsilon_{\mathbf{p}} \alpha_{\mathbf{p}}^2}{1 - \alpha_{\mathbf{p}}^2} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \right). \end{aligned} \quad (3.61)$$

By a suitable choice of $\alpha_{\mathbf{p}}$ and $\epsilon_{\mathbf{p}}$, we can thus recover \mathbb{H}_N . More precisely, we get

$$\alpha_{\mathbf{p}} := \frac{|\mathbf{p}|^2 + g_N \widehat{v}\left(\frac{\mathbf{p}}{N^\beta}\right) - \sqrt{|\mathbf{p}|^2 \left(|\mathbf{p}|^2 + 2g_N \widehat{v}\left(\frac{\mathbf{p}}{N^\beta}\right) \right)}}{g_N \widehat{v}\left(\frac{\mathbf{p}}{N^\beta}\right)}, \quad (3.62)$$

$$\epsilon_{\mathbf{p}} := \sqrt{|\mathbf{p}|^2 \left(|\mathbf{p}|^2 + 2g_N \widehat{v}\left(\frac{\mathbf{p}}{N^\beta}\right) \right)}. \quad (3.63)$$

Now, if we define $\Xi_{\mathbf{p}} := \epsilon_{\mathbf{p}} (1 - \alpha_{\mathbf{p}}^2)^{-1} \alpha_{\mathbf{p}}^2$ and $E_{\text{Bog}} := - \sum_{\mathbf{p} \in \Lambda_+^*} \Xi_{\mathbf{p}}$, we can

finally write

$$\Xi_{\mathbf{p}} = \frac{1}{2} \left[|\mathbf{p}|^2 + g_N \widehat{v} \left(\frac{\mathbf{p}}{N^\beta} \right) - \sqrt{|\mathbf{p}|^2 \left(|\mathbf{p}|^2 + 2g_N \widehat{v} \left(\frac{\mathbf{p}}{N^\beta} \right) \right)} \right], \quad (3.64)$$

$$\mathbb{H}_N = \frac{N-1}{2} g_N \widehat{v}(\mathbf{0}) + E_{\text{Bog}} + \sum_{\mathbf{p} \in \Lambda_+^*} \epsilon_{\mathbf{p}} f_{\mathbf{p}}^\dagger f_{\mathbf{p}} + \frac{1}{N} \sum_{\mathbf{p} \in \Lambda_+^*} \Xi_{\mathbf{p}} a_{\mathbf{p}}^\dagger a_{\mathbf{p}}. \quad (3.65)$$

The value E_{Bog} can be made more explicit.

Lemma 3.2.1. *Let $\nabla \widehat{v}, \frac{\widehat{v}}{|\mathbf{p}|} \in L^1(\mathbb{R}^3)$ and let $d = 3$. Then,*

$$E_{\text{Bog}} = -N^\beta \int_{\mathbb{R}^3} d\mathbf{p} \left(\frac{g_N \widehat{v}(\mathbf{p})}{2|\mathbf{p}|} \right)^2 + o(g_N^2 N^\beta). \quad (3.66)$$

Remark 3.2.2. *A similar formula can also be proven to be true for any dimension $d > 3$, but the same does not happen in $d = 2$; indeed, to have boundedness of the first term on the right side of (3.66) it is required that \widehat{v} vanishes in $\mathbf{0}$. On the other hand, $\widehat{v}(\mathbf{0})$ equals the integral of v and therefore can not vanish under our Assumption 3.0.1.*

Proof. In this proof we denote $\Xi_{\mathbf{p}}$ as $\Xi(\mathbf{p})$ for later convenience. For any $\varphi \in W^{1,1}(\mathbb{R}^3)$ and $M > 0$, we have

$$\left| \int_{\mathbb{R}^3} d\mathbf{p} \varphi(\mathbf{p}) - \frac{1}{M^3} \sum_{\mathbf{p} \in \Lambda_+^*} \varphi\left(\frac{\mathbf{p}}{M}\right) \right| \leq \frac{1}{M^3} \int_{\mathbb{R}^3} d\mathbf{p} |\nabla \varphi(\mathbf{p})|. \quad (3.67)$$

Let us apply the inequality with $M = N^\beta$ and $\Xi(\mathbf{p}) = \varphi\left(\frac{\mathbf{p}}{M}\right)$. Estimating $\nabla [\Xi(N^\beta \mathbf{p})] = N^\beta \nabla \Xi(N^\beta \mathbf{p})$, it is easy to check that

$$\int_{\mathbb{R}^d} d\mathbf{p} \left| N^\beta \nabla \Xi(N^\beta \mathbf{p}) \right| \leq C g_N N^\beta \int_{\mathbb{R}^d} d\mathbf{p} \left(\frac{\widehat{v}(\mathbf{p})}{|\mathbf{p}|} + |\nabla \widehat{v}(\mathbf{p})| \right), \quad (3.68)$$

and applying this to the definition of E_{Bog} , we deduce that

$$\left| E_{\text{Bog}} + N^{d\beta} \int_{\mathbb{R}^d} d\mathbf{p} \Xi(N^\beta \mathbf{p}) \right| \leq C g_N N^\beta. \quad (3.69)$$

It is then straightforward to check that

$$g_N^{-2} N^{2\beta} \int_{\mathbb{R}^d} d\mathbf{p} \Xi(N^\beta \mathbf{p}) = \int_{\mathbb{R}^3} d\mathbf{p} \left(\frac{\widehat{v}}{2|\mathbf{p}|} \right)^2 + o(1), \quad (3.70)$$

which implies the result. □

One expects that in three dimensions E_{Bog} captures the first order correction to the ground state energy

$$E_0(N) = \frac{N-1}{2} g_N \hat{v}(\mathbf{0}) + E_{\text{Bog}} + o\left(g_N^2 N^{(d-2)\beta}\right). \quad (3.71)$$

The main difficulty in proving (3.71) above is that the operators f and f^\dagger do not satisfy the CCRs:

$$[f_{\mathbf{p}}, f_{\mathbf{q}}] = \frac{1}{N \sqrt{(1 - \alpha_{\mathbf{p}}^2)(1 - \alpha_{\mathbf{q}}^2)}} \left(\alpha_{\mathbf{q}} a_{-\mathbf{q}}^\dagger a_{\mathbf{p}} - \alpha_{\mathbf{p}} a_{-\mathbf{p}}^\dagger a_{\mathbf{q}} \right), \quad (3.72)$$

$$[f_{\mathbf{p}}^\dagger, f_{\mathbf{q}}^\dagger] = \frac{1}{N \sqrt{(1 - \alpha_{\mathbf{p}}^2)(1 - \alpha_{\mathbf{q}}^2)}} \left(\alpha_{\mathbf{p}} a_{\mathbf{q}}^\dagger a_{-\mathbf{p}} - \alpha_{\mathbf{q}} a_{\mathbf{p}}^\dagger a_{-\mathbf{q}} \right), \quad (3.73)$$

$$[f_{\mathbf{p}}, f_{\mathbf{q}}^\dagger] = \delta_{\mathbf{p}, \mathbf{q}} \frac{N - \mathcal{N}_+}{N} - \frac{1}{N \sqrt{(1 - \alpha_{\mathbf{p}}^2)(1 - \alpha_{\mathbf{q}}^2)}} \left(a_{\mathbf{q}}^\dagger a_{\mathbf{p}} - \alpha_{\mathbf{p}} \alpha_{\mathbf{q}} a_{-\mathbf{p}}^\dagger a_{-\mathbf{q}} \right). \quad (3.74)$$

A possible strategy to overcome such a difficulty may be to proceed as in [BBCS1] and to exploit a unitary Bogoliubov transformation \mathcal{V} , such that $\mathcal{V} f_{\mathbf{p}} \mathcal{V}^* \approx a_{\mathbf{p}}$, which would lead to estimate the transformed Hamiltonian $\mathcal{V} U_N H_N U_N^* \mathcal{V}$. We do not discuss further this topic and move to the analysis of the dynamical picture.

CHAPTER 4

Dynamics of Bose-Einstein Condensates in the TF Regime

In this last Chapter, we discuss the derivation of an effective equation for a many-body bosonic system in the TF regime. In particular, we prove that, if there is BEC in the initial datum, it is preserved at later times. Based on a joint work in progress with Michele Correggi, David Mitrouskas and Peter Pickl.

4.1 Main Result

We now study the solutions of the N -particle Schrödinger equation

$$\begin{cases} i\partial_t \Psi_t = H_N \Psi_t, \\ \Psi_t|_{t=0} = \Psi_0, \end{cases} \quad (4.1)$$

with symmetric initial state Ψ_0 to be specified below and many-body Hamiltonian H_N given by

$$H_N = \sum_{j=1}^N (-\Delta_j + U(\mathbf{x}_j)) + \frac{g_N}{N} \sum_{1 \leq j < k \leq N} v_N(\mathbf{x}_j - \mathbf{x}_k) \quad (4.2)$$

acting on the Hilbert space $\mathcal{H}_N := \mathfrak{h}^{\otimes_s N}$, with $\mathfrak{h} := L^2(\mathbb{R}^3)$. This describes a trapped system in \mathbb{R}^3 , i.e. what we previously called [Case B](#) in [Section 2.4](#). The trap U is assumed to be a homogeneous potential of the form $U(\mathbf{x}) = k|\mathbf{x}|^s$ with $k > 0$ and $s \geq 2$. In this Chapter, v_N is the intensity of the pair interaction and has the following form.

Assumption 4.1.1. *Let $v \in C_0^\infty(\mathbb{R}^3)$ and $\beta \in (0, 1)$. Then, v_N is given by*

$$v_N(\mathbf{x}) := N^{3\beta} v(N^\beta \mathbf{x}). \quad (4.3)$$

Given the presence of g_N a multiplicative constant in front of the potential we can assume that the integral of v is equal to 1.

Given that H_N is symmetric, the symmetry of the initial datum Ψ_0 is preserved, i.e. it evolves into a symmetric function Ψ_t . Therefore, if we assume that the initial state Ψ_0 shows complete BEC on the one-particle state $\psi_0 \in L^2(\mathbb{R}^3)$, we expect that the many-body state Ψ_t at time t shows BEC as well on a one-particle state ψ_t satisfying the **Gross-Pitaevskii (GP) equation**

$$\begin{cases} i\partial_t \psi_t = \left(-\Delta + U + g_N |\psi_t|^2\right) \psi_t, \\ \psi_t|_{t=0} = \psi_0. \end{cases} \quad (4.4)$$

Our goal is precisely to prove that this guess is asymptotically correct as $N \rightarrow +\infty$.

As we saw already in Section 2.5, due to the presence of $g_N \gg 1$, the kinetic term and the trapping term do not scale in the same way as the interaction term. In particular the minimizer of the effective one-particle problem does not live on a length scale of order 1. A rescaling of the spatial dimensions, and in turn of energy and time, is then called for.

To do that, we define rescaled coordinates \mathbf{y} and time τ introducing new parameters

$$\varepsilon := g_N^{-\frac{s+2}{2(s+3)}}, \quad \tilde{N} := \varepsilon^{-\frac{2}{\beta(s+2)}} N, \quad (4.5)$$

and setting

$$\tau := \varepsilon^{-\frac{2(s+3)}{s+2}} t, \quad \mathbf{y} := \varepsilon^{-\frac{2}{s+2}} \mathbf{x}. \quad (4.6)$$

Remark 4.1.2. Recall that the dilute condition on g_N , as in Proposition 2.5.2, reads $1 \ll g_N \ll N^{\frac{2(s+3)}{3(s+2)}}$. In terms of ε such a condition becomes

$$\varepsilon \gg N^{-\frac{1}{3}}. \quad (4.7)$$

If we then set $\Phi_\tau(\mathbf{y}_1, \dots, \mathbf{y}_N) := g_N^{-\frac{3N}{2(s+3)}} \Psi_t^N(\mathbf{x}_1, \dots, \mathbf{x}_N)$, equation (4.1) becomes

$$\begin{cases} i\partial_\tau \Phi_\tau = K_N \Phi_\tau, \\ \Phi_\tau|_{\tau=0} = \Phi_0^N, \end{cases} \quad (4.8)$$

with a new rescaled Hamiltonian K_N

$$K_N := \sum_{j=1}^N (-\varepsilon^2 \Delta_j + U(\mathbf{y}_j)) + \frac{1}{N} \sum_{1 \leq j < k \leq N} v_{\tilde{N}}(\mathbf{y}_j - \mathbf{y}_k). \quad (4.9)$$

The new Hamiltonian exhibits now two important features: on the one hand, it is now apparent the small pre-factor ε^2 in front of the kinetic term, which plays the role of an effective Planck's constant; on the other hand, the interaction potential now converges to a Dirac delta much faster since $\tilde{N} \gg N$.

The result we wish to prove is that, if we assume factorization in the initial state, then factorization is asymptotically preserved. Hence, we set

$$\phi_\tau(\mathbf{y}) := g_N^{\frac{d}{2(s+d)}} \psi_t(\mathbf{x}), \quad (4.10)$$

so that ϕ_τ now solves the rescaled GP equation

$$\begin{cases} i\partial_\tau \phi_\tau = -\varepsilon^2 \Delta \phi_\tau + U \phi_\tau + |\phi_\tau|^2 \phi_\tau, \\ \phi_\tau|_{\tau=0} = \phi_0. \end{cases} \quad (4.11)$$

To prove our result, a crucial assumption is needed.

Conjecture 4.1.3. *If $\|\phi_0\|_\infty = \mathcal{O}(1)$, then*

$$\sup_{\tau \in [0, +\infty)} \|\phi_\tau\|_\infty \leq C. \quad (4.12)$$

Some comments about the Conjecture above are in order before stating the main result.

Remark 4.1.4. *The statement of Conjecture 4.1.3 does not trivially follow from the properties of the GP equation. Indeed, despite wellposedness is ensured by conservation of the L^2 norm and of the energy, this is not sufficient to prove uniform boundedness of the L^∞ norm, at least in two or more dimensions. Indeed, while in one dimension, conservation of the energy and Sobolev embeddings easily implies the Conjecture, in higher dimension this is not true anymore. On top of that, a second difficulty related to (4.12) is that it requires a uniform estimate of $\|\phi_0\|_\infty$ in terms of the parameter ε , which is typically hard to deduce even knowing a suitable propagation of higher Sobolev norms.*

It is important to notice, however, that even if Conjecture 4.1.3 is crucial for our result, this is mostly a technical problem related to the PDE theory of the GP equation and therefore rather disconnected from the present investigation.

There are however some results toward Conjecture 4.1.3, both in Case A [S12; PTV17] and Case B [C08; C15], but, on the one hand, they do not cover our setting, and, on the other, do not typically provide quantitative estimates of the L^∞ norm, whose dependence on ε is crucial for our result.

For later purposes, it is convenient to introduce an intermediate effective equation, the Hartree equation:

$$\begin{cases} i\partial_\tau \varphi_\tau = -\varepsilon^2 \Delta \varphi_\tau + U \varphi_\tau + v_{\tilde{N}} * |\varphi_\tau|^2 \varphi_\tau \\ \varphi_\tau|_{\tau=0} = \phi_0. \end{cases} \quad (4.13)$$

The result that we aim at proving is then the following

Theorem 4.1.5. *Let $\beta \in (0, \frac{1}{6})$ and $\delta \in (0, 1 - 6\beta)$. If*

$$\|\gamma_{\Psi_0} - P_{\psi_0}\| =: a_N \ll \varepsilon^{-\frac{6}{s+2}} N^{3\beta-1}, \quad (4.14)$$

$$\mathcal{E}^{\text{GP}}[\phi_0] - E^{\text{GP}} =: b_N \ll |\log \varepsilon|^{\frac{3}{4}} \varepsilon^{-\frac{5s+6}{2(s+2)}} N^{-\beta}, \quad (4.15)$$

$$\varepsilon \gg [(1 - 6\beta - \delta) \log N]^{-\frac{s+2}{2(s+3)}}, \quad (4.16)$$

then, for any time $t > 0$,

$$\|\gamma_{\Psi_t} - P_{\psi_t}\| \leq C \varepsilon^{-\frac{6}{s+2}} e^{C\varepsilon^{-\frac{2(s+3)}{s+2}}} N^{-(1-6\beta-\delta)} + C |\log \varepsilon|^{\frac{3}{4}} \varepsilon^{-\frac{13}{4}} N^{-\beta}. \quad (4.17)$$

Remark 4.1.6.

- *The first assumption, (4.14) guarantees that there is BEC in the initial datum; the precise rate in (4.14) allows for the best possible result in (4.17);*
- *the second assumption, (4.15) is a condition on the energy which ensures that the initial datum is close enough to the ground state of the effective problem. This hypothesis is important in particular to prove that the intermediate solution φ_τ is close to ϕ_τ ;*
- *condition (4.16) could actually be dropped from the statement, but it is assumed in order to deduce BEC from (4.17): indeed, we get that for any time $t > 0$*

$$\|\gamma_{\Psi_t} - P_{\psi_t}\| = o(1), \quad (4.18)$$

and therefore there is BEC also at $t > 0$;

- *notice that (4.16) implies (4.7), and therefore the system is dilute in the limit;*
- *the TF scaling is particularly relevant when considering superfluidity features of rotating BECs. In particular, in [JS15] it is shown that if the initial datum has a vortex, then the vortex moves on a time scale of order $t \sim \varepsilon^{\frac{4}{s+2}} |\log \varepsilon|$. Therefore, our result covers the relevant time-scale for the vortex dynamics in BECs. The next step would be to consider an initial many-body state with vortices and study its evolution. Of course, a stronger convergence would be needed, i.e., one would like to prove that for any first order differential operator D ,*

$$\|D(\gamma_{\Psi_t} - P_{\psi_t})\|_{\text{tr}} = o(1). \quad (4.19)$$

The proof is achieved in two steps: first, we use the techniques introduced in [P11] to approximate Φ_τ in terms of φ_τ , and, subsequently, we estimate the distance between φ_τ and ϕ_τ .

4.2 Good and Bad Particles

The key idea about estimating the closeness of Φ_τ to a factorized state is to control the number of *bad particles* in the many-body system (i.e. the particles not in the state φ_τ), using the methods introduced in [P11]. We thus define the projectors on the spaces of good and bad particles and discuss some general properties of these projectors before attacking the derivation of the Hartree equation.

Definition 4.2.1. Let $\varphi \in L^2(\mathbb{R}^3)$ and $\Phi_N \in L^2(\mathbb{R}^{3N})$.

1. For any $1 \leq j \leq N$, the projectors $p_j^\varphi : L^2(\mathbb{R}^{3N}) \rightarrow L^2(\mathbb{R}^{3N})$ and $q_j^\varphi := 1 - p_j^\varphi$ are defined as

$$p_j^\varphi \Phi_N = \varphi(\mathbf{x}_j) \int \varphi^*(\mathbf{z}) \Phi_N(\mathbf{x}_j = \mathbf{z}) d\mathbf{z}. \quad (4.20)$$

2. For any $0 \leq k \leq j \leq N$ we set

$$\mathcal{A}_k^j := \left\{ \mathbf{a} := (a_1, a_2, \dots, a_j) : a_l \in \{0, 1\}, \sum_{l=1}^j a_l = k \right\} \quad (4.21)$$

and define the orthogonal projector $P_{j,k}^\varphi$ on $L^2(\mathbb{R}^{3N})$ as

$$P_{j,k}^\varphi := \sum_{\mathbf{a} \in \mathcal{A}_k^j} \prod_{l=1}^j (p_{N-j+l}^\varphi)^{1-a_l} (q_{N-j+l}^\varphi)^{a_l}. \quad (4.22)$$

In the special case $j = N$, we set $P_k^\varphi := P_{N,k}^\varphi$, while for negative k and $k > j$, we set $P_{j,k}^\varphi := 0$.

3. For any function $f : \{0, 1, \dots, N\} \rightarrow \mathbb{R}_0^+$ we define the operators \widehat{f}^φ and $\widehat{f}_d^\varphi : L^2(\mathbb{R}^{3N}) \rightarrow L^2(\mathbb{R}^{3N})$ as

$$\widehat{f}^\varphi := \sum_{j=0}^N f(j) P_j^\varphi = \sum_{j \in \mathbb{Z}} f(j) P_j^\varphi, \quad (4.23)$$

$$\widehat{f}_d^\varphi := \sum_{j \in \mathbb{Z}} f(j+d) P_j^\varphi. \quad (4.24)$$

Notation 4.2.2. • By comparison to this operator and Lemma 4.2.3, point (b), we can think of \widehat{f}^φ as a different weight on counting the number of particles orthogonal to φ : an estimate on a function f which take a large value on a specific value \bar{k} will be useful to measure \bar{k} particles orthogonal to φ . A natural choice will be to choose to estimate a function f that is larger on higher values of k .

- Observe that the rank of the projector $P_{j,k}^\varphi$ is the space of states that in the last j particles have k good ones.
- We shall also use the bra-ket notation $p_j^\varphi = |\rangle\langle\varphi|_j$ for short.
- Throughout the Chapter hats $\widehat{\cdot}$ shall solely be used in the sense of Definition 4.2.1, part 3.

Some interesting and important properties of the operators defined in Definition 4.2.1 are given in the following Lemma.

Lemma 4.2.3. *Using basic combinatorics of p_j^φ and q_j^φ we get:*

(a) *For any functions $f, g : \{0, 1, \dots, N\} \rightarrow \mathbb{R}_0^+$ we have that*

$$\widehat{f}\widehat{g} = \widehat{f}\widehat{g} = \widehat{g}\widehat{f}, \quad \widehat{f}p_j = p_j\widehat{f}, \quad \widehat{f}P_{j,k} = P_{j,k}\widehat{f}. \quad (4.25)$$

(b) *Let $\nu : \{0, 1, \dots, N\} \rightarrow \mathbb{R}_0^+$ be given by $\nu(k) := \sqrt{\frac{k}{N}}$. Then*

$$(\widehat{\nu}^\varphi)^2 = \frac{1}{N} \sum_{j=1}^N q_j^\varphi, \quad (4.26)$$

i.e., the square of $\widehat{\nu}^\varphi$ is the relative particle number operator of particles not in the state.

(c) *For any $f : \{0, 1, \dots, N\} \rightarrow \mathbb{R}_0^+$ and any symmetric $\Psi \in L^2(\mathbb{R}^{3N})$*

$$\left\| \widehat{f}^\varphi q_1^\varphi \Psi \right\|^2 = \left\| \widehat{f}^\varphi \widehat{\nu}^\varphi \Psi \right\|^2, \quad (4.27)$$

$$\left\| \widehat{f}^\varphi q_1^\varphi q_2^\varphi \Psi \right\|^2 \leq \frac{N}{N-1} \left\| \widehat{f}^\varphi (\widehat{\nu}^\varphi)^2 \Psi \right\|^2. \quad (4.28)$$

(d) *For any $f : \{0, 1, \dots, N\} \rightarrow \mathbb{R}_0^+$, $v : \mathbb{R}^6 \rightarrow \mathbb{R}$ and $j, k = 0, 1, 2$, we have*

$$\widehat{f}^\varphi Q_j^\varphi v(\mathbf{x}_1, \mathbf{x}_2) Q_k^\varphi = Q_j^\varphi v(\mathbf{x}_1, \mathbf{x}_2) \widehat{f}_{j-k}^\varphi Q_k^\varphi, \quad (4.29)$$

where $Q_0^\varphi := p_1^\varphi p_2^\varphi$, $Q_1^\varphi := p_1^\varphi q_2^\varphi$ and $Q_2^\varphi := q_1^\varphi q_2^\varphi$.

Proof. (a) follows immediately from Definition 4.2.1, using that p_j and q_j are orthogonal projectors.

To prove (b) note that $\cup_{k=0}^N \mathcal{A}_k = \{0, 1\}^N$, so that $1 = \sum_{k=0}^N P_k^\varphi$. Using also $(q_k^\varphi)^2 = q_k^\varphi$ and $q_k^\varphi p_k^\varphi = 0$, we get

$$N^{-1} \sum_{k=1}^N q_k^\varphi = N^{-1} \sum_{k=1}^N q_k^\varphi \sum_{j=0}^N P_j^\varphi = N^{-1} \sum_{j=0}^N \sum_{k=1}^N q_k^\varphi P_j^\varphi = N^{-1} \sum_{j=0}^N j P_j^\varphi \quad (4.30)$$

and (b) follows.

Let now $\langle\langle \cdot, \cdot \rangle\rangle$ be the scalar product on $L^2(\mathbb{R}^{3N})$. In order to get (4.27), we can use the symmetry of Ψ and write

$$\left\| \widehat{f}^\varphi \widehat{\nu}^\varphi \Psi \right\|^2 = \langle\langle \Psi, \left(\widehat{f}^\varphi \right)^2 (\widehat{\nu}^\varphi)^2 \Psi \rangle\rangle = N^{-1} \sum_{k=1}^N \langle\langle \Psi, \left(\widehat{f}^\varphi \right)^2 q_k^\varphi \Psi \rangle\rangle = \quad (4.31)$$

$$= \langle\langle \Psi, \left(\widehat{f}^\varphi \right)^2 q_1^\varphi \Psi \rangle\rangle = \langle\langle \Psi, q_1^\varphi \left(\widehat{f}^\varphi \right)^2 q_1^\varphi \Psi \rangle\rangle = \left\| \left(\widehat{f}^\varphi \right) q_1^\varphi \Psi \right\|^2. \quad (4.32)$$

Similarly,

$$\left\| \widehat{f}^\varphi (\widehat{\nu}^\varphi)^2 \Psi \right\|^2 = \langle\langle \Psi, \left(\widehat{f}^\varphi \right)^2 (\widehat{\nu}^\varphi)^4 \Psi \rangle\rangle \quad (4.33)$$

$$= N^{-2} \sum_{j,k=1}^N \langle\langle \Psi, \left(\widehat{f}^\varphi \right)^2 q_j^\varphi q_k^\varphi \Psi \rangle\rangle = \quad (4.34)$$

$$= \frac{N-1}{N} \langle\langle \Psi, \left(\widehat{f}^\varphi \right)^2 q_1^\varphi q_2^\varphi \Psi \rangle\rangle + N^{-1} \langle\langle \Psi, \left(\widehat{f}^\varphi \right)^2 q_1^\varphi \Psi \rangle\rangle = \quad (4.35)$$

$$= \frac{N-1}{N} \left\| \widehat{f}^\varphi q_1^\varphi q_2^\varphi \Psi \right\|^2 + N^{-1} \left\| \widehat{f}^\varphi \widehat{\nu}^\varphi \Psi \right\|^2 \quad (4.36)$$

and (4.28) follows.

Using the definitions above, we also obtain

$$\widehat{f}^\varphi Q_j^\varphi v(\mathbf{x}_1, \mathbf{x}_2) Q_k^\varphi = \sum_{l=0}^N f(l) P_l^\varphi Q_j^\varphi v(\mathbf{x}_1, \mathbf{x}_2) Q_k^\varphi = \quad (4.37)$$

$$= \sum_{l=0}^N f(l) P_{N-2,l-j}^\varphi Q_j^\varphi v(\mathbf{x}_1, \mathbf{x}_2) Q_k^\varphi = \quad (4.38)$$

$$= \sum_{l=0}^N f(l) Q_j^\varphi v(\mathbf{x}_1, \mathbf{x}_2) Q_k^\varphi P_{N-2,l-j}^\varphi = \quad (4.39)$$

$$= \sum_{l=0}^N f(l) Q_j^\varphi v(\mathbf{x}_1, \mathbf{x}_2) Q_k^\varphi P_{l-j+k}^\varphi = \quad (4.40)$$

$$= \sum_{l=k-j}^{N+k-j} Q_j^\varphi v(\mathbf{x}_1, \mathbf{x}_2) f(l+j-k) Q_k^\varphi P_l^\varphi = \quad (4.41)$$

$$= Q_j^\varphi v(\mathbf{x}_1, \mathbf{x}_2) Q_k^\varphi \widehat{f}_{j-k}^\varphi \quad (4.42)$$

which yields (d).

□

4.3 Preliminary Energy Estimates

Before stating and proving the main theorem, we first show some preliminary energy estimates for the GP and Hartree solutions. In general we have that the flow induced by the differential equations (4.11) and (4.13) conserves the energies \mathcal{E}^{GP} and \mathcal{E}^{H} , respectively, where

$$\mathcal{E}^{\text{H}}[\varphi] := \int_{\mathbb{R}^3} d\mathbf{y} \left\{ \varepsilon^2 |\nabla \varphi(\mathbf{y})|^2 + U(\mathbf{y}) |\varphi(\mathbf{y})|^2 + \frac{1}{2} v_{\tilde{N}} * |\varphi|^2(\mathbf{y}) |\varphi(\mathbf{y})|^2 \right\}, \quad (4.43)$$

$$\mathcal{E}^{\text{GP}}[\phi] := \int_{\mathbb{R}^3} d\mathbf{y} \left\{ \varepsilon^2 |\nabla \phi(\mathbf{y})|^2 + U(\mathbf{y}) |\phi(\mathbf{y})|^2 + \frac{1}{2} |\phi(\mathbf{y})|^4 \right\}, \quad (4.44)$$

$$\mathcal{E}^{\text{TF}}[\rho] := \int_{\mathbb{R}^3} d\mathbf{y} \left\{ U(\mathbf{y}) \rho(\mathbf{y}) + \frac{1}{2} \rho^2(\mathbf{y}) \right\}. \quad (4.45)$$

We now want to establish some relations between these three energy functionals and, in particular, between the energies of the states ϕ_τ and φ_τ . We first prove that a energy estimate of the initial state guarantees a control of the kinetic energy at later times. We define the respective ground state energies as

$$E^\# := \inf \left\{ \mathcal{E}^\#[\psi] : \psi \in \mathfrak{h}, \|\psi\| = 1 \right\}. \quad (4.46)$$

We also recall a result proven in [BCPY08].

Theorem 4.3.1 (Bru, Correggi, Pickl, Yngvason, 2008). *Let E^{GP} and E^{TF} be defined as in (4.46). Then,*

$$E^{\text{GP}} = E^{\text{TF}} + \mathcal{O}(\varepsilon |\log \varepsilon|). \quad (4.47)$$

From the previous Theorem, one easily deduces that the kinetic energy of the minimizer $\|\nabla \phi^{\text{GP}}\|^2$ is at most of order $\mathcal{O}(\varepsilon^{-1} |\log \varepsilon|)$; on the other hand, it is easy to show that $\|\nabla \phi^{\text{GP}}\|^2 > C > 0$, where C does not depend on ε .

Proposition 4.3.2. *Let $\phi \in \mathfrak{h}$ be such that*

$$\mathcal{E}^{\text{GP}}[\phi] \leq E^{\text{TF}} + K, \quad \|\phi\| = 1. \quad (4.48)$$

Then, the kinetic energy of ϕ is bounded as

$$\|\nabla \phi\|^2 \leq \frac{K}{\varepsilon^2}. \quad (4.49)$$

Let also ϕ_0 satisfy (4.48), $\|\phi_0\|_\infty$ and Conjecture 4.1.3. Then, if φ_τ is a solution of (4.13), as $N \rightarrow +\infty$

$$\|\nabla \varphi_\tau\|^2 \leq C \frac{\sqrt{K}}{\varepsilon^2} \left(\sqrt{K} + \frac{1}{\tilde{N}^\beta \varepsilon} \right), \quad \forall \tau > 0. \quad (4.50)$$

Finally, let $K \gg \tilde{N}^{-2\beta} \varepsilon^{-2}$, then

$$|\mathcal{E}^{\text{GP}}[\varphi_\tau] - \mathcal{E}^{\text{GP}}[\phi_0]| \leq \frac{C\sqrt{K}}{\tilde{N}^\beta \varepsilon} \left(1 + \frac{K^{\frac{3}{2}}}{\varepsilon^3} \right). \quad (4.51)$$

Proof. From the definitions (4.44) and (4.45) we get

$$\|\nabla \varphi\|^2 = \frac{1}{\varepsilon^2} \left(\mathcal{E}^{\text{GP}}[\varphi] - \mathcal{E}^{\text{TF}}[|\varphi|^2] \right) \leq \frac{1}{\varepsilon^2} \left(\mathcal{E}^{\text{GP}}[\varphi] - E^{\text{TF}} \right) \leq \frac{K}{\varepsilon^2}, \quad (4.52)$$

and this proves (4.49).

To prove (4.50) we use conservation of the energy to write

$$\|\nabla \varphi_\tau\|^2 = \frac{1}{\varepsilon^2} \left(\mathcal{E}^{\text{H}}[\phi_0] - \mathcal{E}^{\text{GP}}[\phi_0] + \mathcal{E}^{\text{GP}}[\phi_0] - \mathcal{E}^{\text{TF}}[|\varphi_\tau|^2] \right) \leq \quad (4.53)$$

$$\leq \frac{1}{\varepsilon^2} \left(|\mathcal{E}^{\text{H}}[\phi_0] - \mathcal{E}^{\text{GP}}[\phi_0]| + |\mathcal{E}^{\text{GP}}[\phi_0] - E^{\text{TF}}| \right). \quad (4.54)$$

The difference between the two energies can be estimated using the fact that the potential converges to a Dirac delta as $\tilde{N} \rightarrow +\infty$. We get that for a generic function ϕ , it holds

$$|\mathcal{E}^{\text{GP}}[\phi] - \mathcal{E}^{\text{H}}[\phi]| = \frac{1}{2} \left| \int_{\mathbb{R}^3} d\mathbf{y} \left[|\phi(\mathbf{y})|^2 - v_{\tilde{N}} * |\phi|^2(\mathbf{y}) \right] |\phi(\mathbf{y})|^2 \right| = \quad (4.55)$$

$$= \frac{1}{2} \left| \int_{\mathbb{R}^6} d\mathbf{y} d\mathbf{z} |\phi(\mathbf{y})|^2 v(\mathbf{z}) \left[|\phi(\mathbf{y})|^2 - \left| \phi\left(\mathbf{y} - \frac{\mathbf{z}}{\tilde{N}^\beta}\right) \right|^2 \right] \right| = \quad (4.56)$$

$$= \frac{1}{2} \left| \int_{\mathbb{R}^6} d\mathbf{y} d\mathbf{z} v(\mathbf{z}) |\phi(\mathbf{y})|^2 \int_0^1 ds \frac{\partial}{\partial s} \left| \phi\left(\mathbf{y} - \frac{s\mathbf{z}}{\tilde{N}^\beta}\right) \right|^2 \right| \leq \quad (4.57)$$

$$\leq \int_0^1 ds \int_{\mathbb{R}^6} d\mathbf{y} d\mathbf{z} \frac{|\mathbf{z}|}{\tilde{N}^\beta} v(\mathbf{z}) |\phi(\mathbf{y})|^2 \left| \phi\left(\mathbf{y} - \frac{s\mathbf{z}}{\tilde{N}^\beta}\right) \right| \left| \nabla \phi\left(\mathbf{y} - \frac{s\mathbf{z}}{\tilde{N}^\beta}\right) \right| \leq \quad (4.58)$$

$$\leq \frac{1}{\tilde{N}^\beta} \int_{\mathbb{R}^3} d\mathbf{z} |\mathbf{z}| v(\mathbf{z}) \|\phi\|_6^3 \|\nabla \phi\| \leq \frac{C}{\tilde{N}^\beta} \|\phi\|_6^3 \|\nabla \phi\|, \quad (4.59)$$

where in the second to last step we used Hölder inequality.

Now we can choose to bound $\|\phi\|_6^3$ in two different ways; either we use a bound on the L^∞ norm of ϕ to get

$$\|\phi\|_6^3 \leq \|\phi\|_\infty^2, \quad (4.60)$$

or we use Sobolev embedding (see [AF03]) to get $\|\phi\|_6^3 \leq C \|\phi\|_{H^1}^3$. The first inequality allows us to estimate the terms containing the difference of energies in (4.54):

$$|\mathcal{E}^{\text{GP}}[\phi_0] - \mathcal{E}^{\text{H}}[\phi_0]| \leq \frac{C}{\tilde{N}^\beta} \|\phi_0\|_\infty^2 \|\nabla \phi_0\| \leq \frac{C\sqrt{K}}{\tilde{N}^\beta \varepsilon} \|\phi_0\|_\infty^2. \quad (4.61)$$

We then substitute this term in (4.54) to finally get

$$\|\nabla \varphi_\tau\|^2 \leq \frac{C}{\varepsilon^2} \left(\frac{\sqrt{K}}{\tilde{N}^\beta \varepsilon} \|\phi_0\|_\infty^2 + K \right) = \frac{C\sqrt{K}}{\tilde{N}^\beta \varepsilon^3} \|\phi_0\|_\infty^2 + \frac{CK}{\varepsilon^2} \quad (4.62)$$

and this concludes the proof of (4.50).

To prove (4.51), notice that, assuming $K \gg \tilde{N}^{-2\beta} \varepsilon^{-2}$, we obtain $\|\nabla \varphi_\tau\|^2 \leq \frac{CK}{\varepsilon^2}$ thanks to Conjecture 4.1.3 and the hypotheses on the initial datum. Using the same calculation above, we then get

$$|\mathcal{E}^{\text{GP}}[\varphi_\tau] - \mathcal{E}^{\text{GP}}[\phi_0]| \leq |\mathcal{E}^{\text{GP}}[\varphi_\tau] - \mathcal{E}^{\text{H}}[\varphi_\tau]| + \quad (4.63)$$

$$+ |\mathcal{E}^{\text{GP}}[\phi_0] - \mathcal{E}^{\text{H}}[\phi_0]| \leq \quad (4.64)$$

$$\leq \frac{C}{\tilde{N}^\beta} \|\varphi_\tau\|_{H^1}^3 \|\nabla \varphi_\tau\| + \frac{C\sqrt{K}}{\tilde{N}^\beta \varepsilon} \|\phi_0\|_\infty^2 \leq \quad (4.65)$$

$$\leq \frac{C\sqrt{K}}{\tilde{N}^\beta \varepsilon} \left(1 + \frac{K^{\frac{3}{2}}}{\varepsilon^3} \right), \quad (4.66)$$

where we have made use of the inequality (4.59), of the hypotheses and of Conjecture 4.1.3.

□

Corollary 4.3.3. *Let φ_τ and ϕ_τ as in (4.13) and (4.4), respectively. Let also ϕ_0 be such that $\mathcal{E}^{\text{GP}}[\phi_0] \leq E^{\text{GP}} + \xi$. Then,*

$$\left\| |\varphi_\tau|^2 - |\phi_\tau|^2 \right\|^2 \leq \frac{C\xi^2}{\tilde{N}^\beta \varepsilon^4} + \frac{C|\log \varepsilon|^{\frac{3}{2}}}{\tilde{N}^\beta \varepsilon^{\frac{5}{2}}} + C\xi. \quad (4.67)$$

Proof. Recall that ϕ^{GP} satisfies

$$-\varepsilon^2 \Delta \phi^{\text{GP}} + U \phi^{\text{GP}} + |\phi^{\text{GP}}|^2 \phi^{\text{GP}} = \mu^{\text{GP}} \phi^{\text{GP}}, \quad (4.68)$$

$$\mu^{\text{GP}} = E^{\text{GP}} + \frac{1}{2} \|\phi^{\text{GP}}\|_4^4. \quad (4.69)$$

Let now $\phi \in \mathfrak{h}$; define $u := \frac{\phi}{\phi^{\text{GP}}}$ (which is well defined because $\phi^{\text{GP}}(\mathbf{x}) > 0$ for any $\mathbf{x} \in L^2(\mathbb{R}^3)$). Then, if we consider the kinetic energy of ϕ , we get

$$\|\nabla \phi\|^2 \geq \|u \nabla \phi^{\text{GP}}\|^2 + \frac{1}{2} \langle \nabla |\phi^{\text{GP}}|^2, \nabla |u|^2 \rangle = -\langle \phi^{\text{GP}}, |u|^2 \Delta \phi^{\text{GP}} \rangle = \quad (4.70)$$

$$= \frac{1}{\varepsilon^2} E^{\text{GP}} + \frac{1}{2\varepsilon^2} \|\phi^{\text{GP}}\|_4^4 - \frac{1}{\varepsilon^2} \langle \phi, (U + |\phi^{\text{GP}}|^2) \phi \rangle. \quad (4.71)$$

Using the inequality above to replace the kinetic energy in $\mathcal{E}^{\text{GP}}[\phi]$, we get

$$\mathcal{E}^{\text{GP}}[\phi] - E^{\text{GP}} \geq \frac{1}{2} \left\| |\phi|^2 - |\phi^{\text{GP}}|^2 \right\|^2. \quad (4.72)$$

We now want to use Proposition 4.3.2; to do so, we notice that hypotheses $\mathcal{E}^{\text{GP}}[\phi_0] \leq E^{\text{GP}} + \xi$ and Theorem 4.3.1 imply that we can choose to apply equation (4.51) with $K \leq \xi + \mathcal{O}(\varepsilon \log \varepsilon)$. Using this information, conservation of \mathcal{E}^{GP} for φ_τ and the previous inequality we get that the distance between $|\phi_\tau|^2$ and $|\varphi_\tau|^2$ can be estimate by showing that are both close to $|\phi^{\text{GP}}|^2$:

$$\left\| |\phi_\tau|^2 - |\varphi_\tau|^2 \right\| \leq \left\| |\phi_\tau|^2 - |\phi^{\text{GP}}|^2 \right\| + \left\| |\varphi_\tau|^2 - |\phi^{\text{GP}}|^2 \right\| \leq \quad (4.73)$$

$$\leq \sqrt{2(\mathcal{E}^{\text{GP}}[\phi_0] - E^{\text{GP}})} + \sqrt{2(\mathcal{E}^{\text{GP}}[\varphi_\tau] - E^{\text{GP}})} \leq \quad (4.74)$$

$$\leq \frac{C\xi}{\tilde{N}^{\frac{\beta}{2}}\varepsilon^2} + \frac{C|\log \varepsilon|^{\frac{3}{4}}}{\tilde{N}^{\frac{\beta}{2}}\varepsilon^{\frac{5}{4}}} + C\sqrt{\xi}. \quad (4.75)$$

□

4.4 Derivation of the Mean-Field Equation

We now discuss the approximation of Φ_τ by the tensor product of one-particle states φ_τ . Proceeding as in [P11] we aim at controlling the functional $\alpha : L^2(\mathbb{R}^{3N}) \times L^2(\mathbb{R}^3) \rightarrow \mathbb{R}_0^+$ given by

$$\alpha(\Phi, \varphi) = \langle \Phi, \widehat{\mu}^\varphi \Phi \rangle \quad (4.76)$$

for some appropriate weight $m : \{0, \dots, N\} \rightarrow \mathbb{R}_0^+$. We prove later that for a suitable choice of m the estimate of $\alpha(\Phi_\tau, \varphi_\tau)$ implies condensation. More precisely, we make the following choice for m .

Definition 4.4.1. For any $\lambda \in (0, 1)$ we define the function μ^λ as

$$\mu^\lambda(k) := \begin{cases} \frac{k}{N^\lambda}, & \text{for } k \leq N^\lambda \\ 1, & \text{otherwise.} \end{cases} \quad (4.77)$$

Moreover, for any $N \in \mathbb{N}$, we define the functional $\alpha_N^\lambda : L^2(\mathbb{R}^{3N}) \times L^2(\mathbb{R}^3) \rightarrow \mathbb{R}_0^+$ as

$$\alpha_N^\lambda(\Phi, \phi) := \langle \Phi, \hat{\mu}^{\lambda, \phi} \Phi \rangle = \left\| \left(\hat{\mu}^{\lambda, \phi} \right)^{1/2} \Phi \right\|^2. \quad (4.78)$$

We are now able to state the result that provides the first part of the proof of Theorem 4.1.5.

Theorem 4.4.2. *Let $\beta \in (0, \frac{1}{6})$ and $\lambda \in (3\beta, 1 - 3\beta)$. Let also $v_N(\mathbf{x})$ satisfy Assumption 4.1.1, then*

$$\begin{aligned} \alpha_N^\lambda(\Phi_\tau, \varphi_\tau) &\leq \\ &\leq \frac{\varepsilon^{-\frac{6}{s+2}} N^{3\beta-\lambda}}{\left(1 + \varepsilon^{-\frac{3}{s+2}} N^{-\frac{1-\lambda-3\beta}{2}}\right)} \left(e^{\left(1 + \varepsilon^{-\frac{3}{s+2}} N^{-\frac{1-\lambda-3\beta}{2}}\right)\tau} - 1 \right) + \\ &\quad + \alpha_N^\lambda(\Phi_0, \phi_0) e^{\left(1 + \varepsilon^{-\frac{3}{s+2}} N^{-\frac{1-\lambda-3\beta}{2}}\right)\tau}. \end{aligned} \quad (4.79)$$

Corollary 4.4.3. *If $\left\| \gamma_{\Phi_\tau}^{(1)} - P_{\psi_\tau} \right\| \leq \xi$ for some $\xi = o(1)$, and*

$$\varepsilon^{-\frac{3}{s+2}} N^{-\frac{1-\lambda-3\beta}{2}} \ll 1 \quad (4.80)$$

$$\eta_N := \max \left\{ \varepsilon^{-\frac{6}{s+2}} N^{3\beta-1}, \xi \right\}, \quad (4.81)$$

then for any fixed time τ

$$\left\| \gamma^{\Phi_\tau} - P_{\varphi_\tau} \right\|_1 \leq C \eta_N N^{1-\lambda} e^{C\tau} \left(1 + \eta_N N^{1-\lambda} e^{C\tau} \right). \quad (4.82)$$

Proof of the Corollary. We first use Lemma 4.4.4 to get that $\alpha_N^\lambda(\Phi_0, \phi_0) \leq \mathcal{O}(\xi N^{1-\lambda})$; we then apply Theorem 4.4.2 and use the hypotheses to get that

$$\alpha_N^\lambda(\Phi_\tau, \varphi_\tau) \leq \left(\varepsilon^{-\frac{6}{s+2}} N^{3\beta-\lambda} + \mathcal{O}(\xi N^{1-\lambda}) \right) e^{C\tau} \leq \quad (4.83)$$

$$\leq C \max \left\{ \varepsilon^{-\frac{6}{s+2}} N^{3\beta-1}, \xi \right\} N^{1-\lambda} e^{C\tau}. \quad (4.84)$$

We now estimate the difference between the projectors:

$$\left\| \gamma^{\Phi_\tau} - P_{\varphi_\tau} \right\|_1 \leq 2 \|q_1 \varphi_\tau\| (1 + \|q_1 \varphi_\tau\|). \quad (4.85)$$

Now, q_1 can be bounded in terms of α_N^λ as

$$\|q_1 \varphi_\tau\|^2 \leq \langle \Phi_\tau, \hat{\mu}^{\lambda, \phi_\tau} \Phi_\tau \rangle = \alpha_N^\lambda(\Phi_\tau, \phi_\tau) \leq \quad (4.86)$$

$$\leq \max \left\{ \varepsilon^{-\frac{6}{s+2}} N^{3\beta-1}, \xi \right\} N^{1-\lambda} e^{C\tau} \quad (4.87)$$

and the result follows. □

4.4.1 Convergence of the Reduced Density Matrix

In [P11] it is shown that if $\mu \equiv \nu^2 = \frac{k}{N}$ then convergence of $\alpha(\Phi, \phi)$ to 0 is equivalent to convergence in trace norm of the 1-reduced density matrix to P_ϕ . In our case the two convergences are not equivalent, but we remark here that since $\mu^\lambda(k) \geq \frac{k}{N}$, for all $0 \leq k \leq N$ and all $\lambda \in (0, 1)$, then $\alpha_N^\lambda(\Phi, \phi) \geq \langle \Phi, \hat{\nu}^2 \Phi \rangle$. Therefore, [P11] implies that, for all $\lambda \in (0, 1)$,

$$\lim_{N \rightarrow +\infty} \alpha_N^\lambda(\Phi, \varphi) = 0 \Rightarrow \lim_{N \rightarrow +\infty} \gamma^\Phi \xrightarrow{\|\cdot\|} P_\varphi \text{ in operator norm.} \quad (4.88)$$

The converse is not true and thus to deduce condensation from the estimate of $\alpha_N^\lambda(\Phi_0, \phi_0)$ and the condensation assumption at initial time, we need the following Lemma.

Lemma 4.4.4. *Let $0 < \lambda < 1$, $\xi < 0$ and let $\|\gamma^\Phi - P_\phi\| = o(N^\xi)$. Then*

$$\alpha_N^\lambda(\Phi, \phi) = o(N^{1-\lambda+\xi}). \quad (4.89)$$

Proof. Under the above assumptions, $\langle \phi, \gamma^\Phi \phi \rangle = o(N^\xi)$. Writing

$$\begin{aligned} \alpha^\Phi &= \int \Phi(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N) \bar{\Phi}(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N) d\mathbf{x} \\ &= \int \left(p_1^\phi \Phi\right)(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N) \left(p_1^\phi \bar{\Phi}\right)(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N) d\mathbf{x} + \\ &+ \int \left(q_1^\phi \Phi\right)(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N) \left(p_1^\phi \bar{\Phi}\right)(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N) d\mathbf{x} + \\ &+ \int \left(p_1^\phi \Phi\right)(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N) \left(q_1^\phi \bar{\Phi}\right)(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N) d\mathbf{x} + \\ &+ \int \left(q_1^\phi \Phi\right)(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N) \left(q_1^\phi \bar{\Phi}\right)(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N) d\mathbf{x} \end{aligned}$$

and using that $(q_1^\phi \phi)(\mathbf{x}_1) = 0$, we obtain that $\|p_1^\phi \Phi\|^2 - 1 = o(N^\xi)$. By the identity $p_1^\phi + q_1^\phi = 1$ and Lemma 4.2.3, point (c),

$$\|q_1^\phi \Phi\|^2 = \langle \Phi, \hat{\nu}^2 \Phi \rangle = \left\langle \Phi, \sum_{k=0}^N \frac{k}{N} P_k^\phi \Phi \right\rangle = o(N^\xi). \quad (4.90)$$

Since $\mu^\lambda(k) \leq kN^{-\lambda}$, for any $0 \leq k \leq N$,

$$\alpha_N^\lambda(\Phi, \phi) \leq N^{1-\lambda} \left\langle \Phi, \sum_{k=0}^N \frac{k}{N} P_k^\phi \Phi \right\rangle = o(N^{1-\lambda+\xi}). \quad (4.91)$$

□

4.4.2 Proof of Theorem 4.4.2

We first state some useful operator estimates.

Proposition 4.4.5. (a) For any $f \in L^2(\mathbb{R}^3)$ and for any $a \in [1, +\infty]$

$$\left\| f(\mathbf{x}_1 - \mathbf{x}_2) p_1^\phi \right\| \leq \|\phi\|_{2a} \|f\|_{2a'} . \quad (4.92)$$

(b) For any $g \in L^1(\mathbb{R}^3)$ and for any $b \in [1, +\infty]$

$$\left\| p_1^\phi g(\mathbf{x}_1 - \mathbf{x}_2) p_1^\phi \right\| \leq \|\phi\|_{2b}^2 \|g\|_{b'} . \quad (4.93)$$

(c) Let v_N be defined as in (4.3). Then,

$$\|v_N\|_p = N^{\frac{3\beta}{p'}} \|v\|_p \quad (4.94)$$

Proof. The proof of (c) follows from a simple calculation and we omit it. We then focus on the proofs of (a) and (b).

We start with (a): setting $p_1^\phi = |\phi(\mathbf{x}_1)\rangle\langle\phi(\mathbf{x}_1)|$, we get

$$\left\| f(\mathbf{x}_1 - \mathbf{x}_2) p_1^\phi \right\|^2 = \sup_{\|\Phi\|=1} \left\| f(\mathbf{x}_1 - \mathbf{x}_2) p_1^\phi \Phi \right\|^2 \quad (4.95)$$

$$= \sup_{\|\Phi\|=1} \langle\langle \Phi, |\phi(\mathbf{x}_1)\rangle\langle\phi(\mathbf{x}_1)| f^2(\mathbf{x}_1 - \mathbf{x}_2) |\phi(\mathbf{x}_1)\rangle\langle\phi(\mathbf{x}_1)| \Phi \rangle\rangle. \quad (4.96)$$

Using that for any given $a \in [1, +\infty]$

$$\sup_{\mathbf{x}_2 \in \mathbb{R}^3} \langle\phi(\mathbf{x}_1)| f^2(\mathbf{x}_1 - \mathbf{x}_2) |\phi(\mathbf{x}_1)\rangle \leq \|\phi\|_{2a}^2 \|f\|_{2a'}^2 \quad (4.97)$$

and applying Cauchy-Schwarz inequality, one gets

$$\left\| f(\mathbf{x}_1 - \mathbf{x}_2) p_1^\phi \right\|^2 \leq \sup_{\|\Phi\|=1} \|\Phi\|^2 \|\phi\|_{2a}^2 \|f\|_{2a'}^2 . \quad (4.98)$$

To prove (b), we estimate

$$\left\| p_1^\phi g(\mathbf{x}_1 - \mathbf{x}_2) p_1^\phi \right\| \leq \left\| p_1^\phi |g(\mathbf{x}_1 - \mathbf{x}_2)| p_1^\phi \right\| \quad (4.99)$$

$$= \left\| p_1^\phi \sqrt{|g(\mathbf{x}_1 - \mathbf{x}_2)|} \sqrt{|g(\mathbf{x}_1 - \mathbf{x}_2)|} p_1^\phi \right\| \quad (4.100)$$

$$\leq \left\| \sqrt{|g(\mathbf{x}_1 - \mathbf{x}_2)|} p_1^\phi \right\|^2 , \quad (4.101)$$

and by (a), we get (b).

□

We now want to apply a Grönwall-type argument to estimate the growth in time of $\alpha_N^\lambda(\Phi_\tau, \varphi_\tau)$, and therefore we need to study $\dot{\alpha}_N^\lambda(\Phi_\tau, \varphi_\tau)$. We use the following definitions to simplify notation.

Definition 4.4.6. We denote by $U_{j,k}$ the difference between the time and mean-field interactions for two particles, i.e.

$$U_{j,k} := (N-1) v_{\tilde{N}}(\mathbf{x}_j - \mathbf{x}_k) - N v_{\tilde{N}} * |\varphi_\tau|^2(\mathbf{x}_j) - N v_{\tilde{N}} * |\varphi_\tau|^2(\mathbf{x}_k). \quad (4.102)$$

Lemma 4.4.7. Let $\Gamma_N^\lambda : L^2(\mathbb{R}^{3N}) \rightarrow \mathbb{R}$ be defined as

$$\Gamma_N^\lambda(\Phi, \varphi) := 2\text{Im} \left(\langle \Phi, \left(\hat{\mu}_{-1}^{\lambda, \varphi} - \hat{\mu}^{\lambda, \varphi} \right) p_1 q_2 U_{1,2} p_1 p_2 \Phi \rangle \right) \quad (4.103)$$

$$+ \text{Im} \left(\langle \Phi, q_1 q_2 U_{1,2} \left(\hat{\mu}^{\lambda, \varphi} - \hat{\mu}_2^{\lambda, \varphi} \right) p_1 p_2 \Phi \rangle \right) \quad (4.104)$$

$$+ 2\text{Im} \left(\langle \Phi, \left(\hat{\mu}_{-1}^{\lambda, \varphi} - \hat{\mu}^{\lambda, \varphi} \right) q_1 q_2 U_{1,2} p_1 q_2 \Phi \rangle \right). \quad (4.105)$$

Then, for any solutions Φ_τ and φ_τ of the Schrödinger (4.8) and mean-field (4.11) equations respectively, and for any $\lambda \in (0, 1)$, we have

$$\dot{\alpha}_N^\lambda(\Phi_\tau, \varphi_\tau) = \Gamma_N^\lambda(\Phi_\tau, \varphi_\tau). \quad (4.106)$$

Proof. Let

$$H_{mf}^\varphi := \sum_{j=1}^N [-\varepsilon^2 \Delta + U + v_{\tilde{N}} * |\varphi|^2(\mathbf{x}_j)] \quad (4.107)$$

be the sum of mean-field Hamiltonians. We have

$$\frac{d}{d\tau} \hat{f}^{\varphi_\tau} = i \left[\hat{f}^{\varphi_\tau}, H_{mf}^{\varphi_\tau} \right] \quad (4.108)$$

for any function $f : \{0, \dots, N\} \rightarrow \mathbb{R}$. We will now drop the labels φ_τ and λ in the rest of the proof to simplify the notation. By (4.108), we get

$$\dot{\alpha}_N^\lambda(\Phi_\tau, \varphi_\tau) = i \langle \Phi_\tau, K_N \Phi_\tau, \hat{\mu} \Phi_\tau \rangle - i \langle \Phi_\tau, \hat{\mu} K_N \Phi_\tau \rangle + i \langle \Phi_\tau, [\hat{\mu}, H_{mf}] \Phi_\tau \rangle \quad (4.109)$$

$$= i \langle \Phi_\tau, [K_N - H_{mf}, \hat{\mu}] \Phi_\tau \rangle. \quad (4.110)$$

Using the symmetry of Φ_τ and the selfadjointness of $U_{j,k}$, we obtain

$$\begin{aligned} \dot{\alpha}_N^\lambda(\Phi_\tau, \varphi_\tau) &= \frac{i}{2} \langle \Phi_\tau, [U_{1,2}, \hat{\mu}] \Phi_\tau \rangle \\ &= \frac{1}{2i} (\langle \Phi_\tau, \hat{\mu} U_{1,2} \Phi_\tau \rangle - \langle \Phi_\tau, U_{1,2} \hat{\mu} \Phi_\tau \rangle) \\ &= \text{Im} (\langle \Phi_\tau, \hat{\mu} U_{1,2} \Phi_\tau \rangle). \end{aligned} \quad (4.111)$$

Note that, for any $\mu : \{1, \dots, N\} \rightarrow \mathbb{R}_0^+$ (remember that $P_{N,k} = 0$ whenever $k < 0$ or $k > N$), we can write

$$\begin{aligned}
\hat{\mu} &= \sum_{k=0}^N \mu(k) P_k \\
&= \sum_{k=0}^{N-2} (\mu(k) p_1 p_2 P_{N-2,k} + \mu(k) p_1 q_2 P_{N-2,k-1} \\
&\quad + \mu(k) q_1 p_2 P_{N-2,k-1} + \mu(k) (1 - p_1 q_2 - q_1 p_2 - p_1 p_2) P_{N-2,k-2}) \\
&= \sum_{k=0}^N (\mu(k) p_1 p_2 P_{N-2,k} + \mu(k) p_1 q_2 P_{N-2,k-1} \\
&\quad + \mu(k) q_1 p_2 P_{N-2,k-1} + \mu(k) P_{N-2,k-2}) \\
&\quad - \sum_{k=0}^N (\mu(k+1) p_1 q_2 P_{N-2,k-1} + \mu(k+1) q_1 p_2 P_{N-2,k-1} \\
&\quad + \mu(k+2) p_1 p_2 P_{N-2,k}) \\
&= (\hat{\mu} - \hat{\mu}_2) p_1 p_2 + (\hat{\mu} - \hat{\mu}_1) p_1 q_2 + (\hat{\mu} - \hat{\mu}_1) q_1 p_2 \\
&\quad + \sum_{k=0}^N m(k) P_{N-2,k-2} .
\end{aligned} \tag{4.112}$$

Using again the symmetry of Φ_τ and the selfadjointness of $U_{1,2} P_{N-2,k-2}$, we also have

$$\dot{\alpha}_N^\lambda(\Phi_\tau, \varphi_\tau) = \text{Im}(\langle \Phi_\tau, U_{1,2} ((\hat{\mu} - \hat{\mu}_2) p_1 p_2 + 2(\hat{\mu} - \hat{\mu}_1) p_1 q_2) \Phi_\tau \rangle) . \tag{4.113}$$

Since $1 = p_1 p_2 + p_1 q_2 + q_1 p_2 + q_1 q_2$

$$\dot{\alpha}_N^\lambda(\Phi_\tau, \varphi_\tau) = \text{Im}(\langle \Phi, p_1 p_2 U_{1,2} (\hat{\mu} - \hat{\mu}_2) p_1 p_2 \Phi \rangle) \tag{4.114}$$

$$+ \text{Im}(\langle \Phi, p_1 q_2 U_{1,2} (\hat{\mu} - \hat{\mu}_2) p_1 p_2 \Phi \rangle) \tag{4.115}$$

$$+ \text{Im}(\langle \Phi, q_1 p_2 U_{1,2} (\hat{\mu} - \hat{\mu}_2) p_1 p_2 \Phi \rangle) \tag{4.116}$$

$$+ \text{Im}(\langle \Phi, q_1 q_2 U_{1,2} (\hat{\mu} - \hat{\mu}_2) p_1 p_2 \Phi \rangle) \tag{4.117}$$

$$+ 2\text{Im}(\langle \Phi, p_1 p_2 U_{1,2} (\hat{\mu} - \hat{\mu}_1) p_1 q_2 \Phi \rangle) \tag{4.118}$$

$$+ 2\text{Im}(\langle \Phi, p_1 q_2 U_{1,2} (\hat{\mu} - \hat{\mu}_1) p_1 q_2 \Phi \rangle) \tag{4.119}$$

$$+ 2\text{Im}(\langle \Phi, q_1 p_2 U_{1,2} (\hat{\mu} - \hat{\mu}_1) p_1 q_2 \Phi \rangle) \tag{4.120}$$

$$+ 2\text{Im}(\langle \Phi, q_1 q_2 U_{1,2} (\hat{\mu} - \hat{\mu}_1) p_1 q_2 \Phi \rangle) . \tag{4.121}$$

Notice that for any operator A if A^* is the adjoint of A , $\text{Im}(\langle \Phi, A\Phi \rangle) = -\text{Im}(\langle \Phi, A^*\Phi \rangle)$. Since Φ is symmetric (note that $p_1 q_2 U_{1,2} q_1 p_2$ is invariant

under adjunction with simultaneous exchange of the variables \mathbf{x}_1 and \mathbf{x}_2) and by Lemma 4.2.3, point (d), we get

$$\begin{aligned} \dot{\alpha}_N^\lambda(\Phi_\tau, \varphi_\tau) &= 2\text{Im}(\langle\langle \Phi, p_1 q_2 U_{1,2}(\widehat{\mu} - \widehat{\mu}_2) p_1 p_2 \Phi \rangle\rangle) \\ &\quad - 2\text{Im}(\langle\langle \Phi, p_1 q_2(\widehat{\mu} - \widehat{\mu}_1) U_{1,2} p_1 p_2 \Phi \rangle\rangle) \end{aligned} \quad (4.122)$$

$$+ \text{Im}(\langle\langle \Phi, q_1 q_2 U_{1,2}(\widehat{\mu} - \widehat{\mu}_2) p_1 p_2 \Phi \rangle\rangle) \quad (4.123)$$

$$+ 2\text{Im}(\langle\langle \Phi, q_1 q_2 U_{1,2}(\widehat{\mu} - \widehat{\mu}_1) p_1 q_2 \Phi \rangle\rangle) . \quad (4.124)$$

The application of Lemma 4.2.3, point (d) applied to the first and second summand completes the proof. \square

If we now manage to estimate $\Gamma_N^\lambda(\Phi_\tau, \varphi_\tau)$ in terms of $\alpha_N^\lambda(\Phi_\tau, \varphi_\tau)$, equation (4.79) will follow from Lemma 4.4.7. This is the content of next Proposition

Proposition 4.4.8. *Let v_N satisfy Assumption 4.1.1. Then,*

$$(a) \quad \left| \langle\langle \Phi, (\widehat{\mu}_{-1}^{\lambda,\varphi} - \widehat{\mu}^{\lambda,\varphi}) p_1 q_2 U_{1,2} p_1 p_2 \Phi \rangle\rangle \right| = 0; \quad (4.125)$$

$$(b) \quad \begin{aligned} &\left| \langle\langle \Phi, q_1 q_2 U_{1,2} (\widehat{\mu}^{\lambda,\varphi} - \widehat{\mu}_2^{\lambda,\varphi}) p_1 p_2 \Phi \rangle\rangle \right| \\ &\leq C \left(\alpha_N^\lambda(\Phi, \varphi) + \varepsilon^{-\frac{6}{s+2}} N^{3\beta-\lambda} \right); \end{aligned} \quad (4.126)$$

$$(c) \quad \begin{aligned} &\left| \langle\langle \Phi, (\widehat{\mu}_{-1}^{\lambda,\varphi} - \widehat{\mu}^{\lambda,\varphi}) q_1 q_2 U_{1,2} p_1 q_2 \Phi \rangle\rangle \right| \\ &\leq C N^{-\frac{1-\lambda}{2}} \alpha_N^\lambda \left(1 + \varepsilon^{-\frac{3}{s+2}} N^{\frac{3\beta}{2}} \right). \end{aligned} \quad (4.127)$$

Before proving Proposition 4.4.8, we comment on points (a) and (c) first: point (a) is in fact the most relevant physical estimate, since the mean-field interaction almost cancels out with the original interaction. The key point is indeed the vanishing of $p_1 q_2 U_{1,2} p_1 p_2$.

For point (c) the choice of the weight μ^λ plays an important role. Note that we have only one projector p here and $\|q_1 q_2 U_{1,2} p_1 q_2\|$ can not be bounded by the L^1 -norm of v . On the other hand, there are three projectors q in (c). Assuming that the condensate is very clean (which is encoded in $\widehat{\mu}^\lambda$), such q 's make (c) small.

Notice however that $\mu^\lambda(k-1) - \mu^\lambda(k-2)$ is approximately the derivative of m with respect to k when N is large, so that $\widehat{\mu}_1^\lambda - \widehat{\mu}_2^\lambda \approx \widehat{k^{-1}m}$. On the other hand, each q yields a factor $\sqrt{\frac{k}{N}}$ (see Lemma 4.2.3, point (c)). Now, the derivative of μ^λ is 0 if $k > N^\lambda$, so we can think as $k \leq N^\lambda$. Thus, the three projectors q appearing in point (c) can heuristically be thought to yield a factor $N^{-\frac{3}{2}(1-\lambda)}$.

Proof. In the proof we shall drop the labels λ and ϕ for short. For any $f : \mathbb{R}^6 \rightarrow \mathbb{R}$

$$\begin{aligned} p_1 f(\mathbf{x}_1 - \mathbf{x}_2) p_1 &= |\phi(\mathbf{x}_1)\rangle \langle \phi(\mathbf{x}_1)| f(\mathbf{x}_1 - \mathbf{x}_2) |\phi(\mathbf{x}_1)\rangle \langle \phi(\mathbf{x}_1)| = \\ &= (f * |\phi|^2)(\mathbf{x}_2) p_1. \end{aligned} \quad (4.128)$$

Using v_N in place of f in (4.128), we obtain

$$p_1 v_{\widetilde{N}}(\mathbf{x}_1 - \mathbf{x}_2) p_1 = [p_1 (v_{\widetilde{N}} * |\phi|^2)](\mathbf{x}_2) p_1. \quad (4.129)$$

Note that p_2 and $(v_{\widetilde{N}} * |\phi|^2)(\mathbf{x}_1)$ commute, thus $p_2 (v_{\widetilde{N}} * |\phi|^2)(\mathbf{x}_1) q_2 = 0$. Hence, from (4.129) we deduce that

$$p_1 p_2 (v_{\widetilde{N}}(\mathbf{x}_1 - \mathbf{x}_2) - v_{\widetilde{N}} * |\phi|^2(\mathbf{x}_1) - v_{\widetilde{N}} * |\phi|^2(\mathbf{x}_2)) p_1 q_2 = 0 \quad (4.130)$$

which proves point (a).

For point (b) we use first that $q_1 q_2 w(\mathbf{x}_1) p_1 p_2 = 0$ for any function w . Then, by Lemma 4.2.3, point (d)

$$\begin{aligned} \langle\langle \Phi, q_1 q_2 U_{1,2}(\widehat{\mu} - \widehat{\mu}_2) p_1 p_2 \Phi \rangle\rangle &= \\ &= (N-1) \langle\langle \Phi, q_1 q_2 (\widehat{\mu}_{-2} - \widehat{\mu})^{1/2} v_{\widetilde{N}}(\mathbf{x}_1 - \mathbf{x}_2) (\widehat{\mu} - \widehat{\mu}_2)^{1/2} p_1 p_2 \Phi \rangle\rangle. \end{aligned} \quad (4.131)$$

Before we estimate this term note that the operator norm of $q_1 q_2 v_{\widetilde{N}}(\mathbf{x}_1 - \mathbf{x}_2)$ restricted to the subspace of symmetric functions is much smaller than its operator norm. This is due to the fact that $v_{\widetilde{N}}(\mathbf{x}_1 - \mathbf{x}_2)$ is nonzero only in a small region where $\mathbf{x}_1 \approx \mathbf{x}_2$, because of compact support of v . A non-symmetric wave function may be fully localized in that area, whereas the same is impossible for a symmetric wave function. To get sufficiently good control of (4.131), we symmetrize $(N-1) v_{\widetilde{N}}(\mathbf{x}_1 - \mathbf{x}_2)$ replacing it with

$\sum_{k=2}^N v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_k)$, and get

$$\begin{aligned}
(4.131) &= (N-1) \langle \Phi, q_1 q_2 (\hat{\mu}_{-2} - \hat{\mu})^{1/2} v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_2) (\hat{\mu} - \hat{\mu}_2)^{1/2} p_1 p_2 \Phi \rangle = \\
&= \langle \Phi, (\hat{\mu}_{-2} - \hat{\mu})^{1/2} \sum_{j=2}^N q_1 q_j v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_j) p_1 p_j (\hat{\mu} - \hat{\mu}_2)^{1/2} \Phi \rangle \\
&\leq \left\| (\hat{\mu}_{-2} - \hat{\mu})^{1/2} q_1 \Phi \right\| \left\| \sum_{j=2}^N q_j v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_j) p_1 p_j (\hat{\mu} - \hat{\mu}_2)^{1/2} \Phi \right\|.
\end{aligned} \tag{4.132}$$

Since

$$\frac{k}{N} (m(k) - m(k-2)) \leq \frac{2}{N} m(k) \tag{4.133}$$

then, in view of Lemma 4.2.3, point (c), we get

$$\left\| (\hat{\mu}_{-2} - \hat{\mu})^{1/2} q_1 \Phi \right\|^2 = \langle \Phi, (\hat{\mu}_{-2} - \hat{\mu}) \hat{\nu}^2 \Phi \rangle \leq \frac{2}{N} \alpha_N^\lambda(\Phi, \phi). \tag{4.134}$$

On the other hand, the second factor of (4.132) squared is bounded by

$$\begin{aligned}
&\frac{1}{2} \sum_{2 \leq j < k \leq N} \langle (\hat{\mu} - \hat{\mu}_2)^{1/2} \Phi, p_1 p_j v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_j) q_j \times \\
&\quad \times q_k v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_k) (\hat{\mu} - \hat{\mu}_2)^{1/2} p_1 p_k \Phi \rangle + \\
&\quad + \sum_{k=2}^N \left\| q_k v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_k) p_1 p_k (\hat{\mu} - \hat{\mu}_2)^{1/2} \Phi \right\|^2.
\end{aligned} \tag{4.135}$$

Using symmetry, Proposition 4.4.5 and (4.94), the first summand in (4.135) is bounded by

$$N^2 \langle (\hat{\mu} - \hat{\mu}_2)^{1/2} \Phi, p_1 p_2 q_3 v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_2) v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_3) p_1 q_2 p_3 (\hat{\mu} - \hat{\mu}_2)^{1/2} \Phi \rangle \tag{4.136}$$

$$\leq N^2 \left\| \sqrt{|v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_2)|} \sqrt{|v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_3)|} p_1 q_2 p_3 (\hat{\mu} - \hat{\mu}_2)^{1/2} \Phi \right\|^2 \tag{4.137}$$

$$\leq N^2 \left\| \sqrt{|v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_2)|} p_1 \right\|^4 \left\| (\hat{\mu} - \hat{\mu}_2)^{1/2} q_2 \Phi \right\|^2 \tag{4.138}$$

$$\leq N^2 \|\phi_\tau\|_\infty^4 \|v_{\tilde{N}}\|_1^2 \left\| (\hat{\mu} - \hat{\mu}_2)^{1/2} q_2 \Phi \right\|^2 \tag{4.139}$$

$$\leq N \|v\|_1^2 \|\phi_\tau\|_\infty^4 \alpha_N^\lambda(\Phi, \phi). \tag{4.140}$$

Analogously, using Proposition 4.4.5 and (4.4.5), point (c), one can control the second summand in (4.135) by

$$N \langle (\hat{\mu} - \hat{\mu}_2)^{1/2} \Phi, p_1 p_2 (v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_2))^2 p_1 p_2 (\hat{\mu} - \hat{\mu}_2)^{1/2} \Phi \rangle \quad (4.141)$$

$$\leq N \left\| p_1 p_2 (v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_2))^2 p_1 p_2 \right\| \left\| (\hat{\mu} - \hat{\mu}_2)^{1/2} \right\|^2 \quad (4.142)$$

$$\leq N \|\phi\|_4^4 \|v_{\tilde{N}}\|^2 \|(\hat{\mu} - \hat{\mu}_2)\| \leq C \varepsilon^{-\frac{2d}{s+2}} N^{1+d\beta-\lambda}. \quad (4.143)$$

By Conjecture 4.1.3, (b) is bounded by

$$C \sqrt{\alpha_N^\lambda(\Phi, \phi)} \sqrt{\alpha_N^\lambda(\Phi, \phi) + \varepsilon^{-\frac{2d}{s+2}} N^{d\beta-\lambda}} \quad (4.144)$$

$$\leq C \left(\alpha_N^\lambda(\Phi, \phi) + \varepsilon^{-\frac{2d}{s+2}} N^{d\beta-\lambda} \right). \quad (4.145)$$

Finally, we prove (c). Using Definition 4.2.1, Proposition 4.4.5, Lemma 4.2.3, point (c) and Cauchy-Schwarz inequality we can estimate the left hand side of (c) as

$$|\langle \Phi, q_1 q_2 U_{1,2} p_1 q_2 (\hat{\mu} - \hat{\mu}_1) \Phi \rangle| \quad (4.146)$$

$$\leq \left\| (\hat{\mu}_{-1} - \hat{\mu})^{1/2} q_1 q_2 \Phi \right\| \left\| U_{1,2} (\hat{\mu} - \hat{\mu}_1)^{1/2} p_1 q_2 \Phi \right\| \quad (4.147)$$

$$\leq \frac{N}{N-1} \left\| (\hat{\mu}_{-1} - \hat{\mu})^{1/2} \hat{\nu}^2 \Phi \right\| \|U_{1,2} p_1\| \left\| (\hat{\mu} - \hat{\mu}_1)^{1/2} \hat{\nu} \Phi \right\|. \quad (4.148)$$

Since

$$m(k) - m(k+1) = \begin{cases} N^{-\lambda}, & \text{if } k \leq N^\lambda, \\ 0, & \text{otherwise,} \end{cases} \quad (4.149)$$

it follows that

$$|m(k-1) - m(k)| \frac{k^2}{N^2} \leq N^{\lambda-2} m(k), \quad (4.150)$$

and thus

$$\left\| (\hat{\mu}_{-1} - \hat{\mu})^{\frac{1}{2}} \hat{\nu}^2 \Phi \right\| \leq N^{\frac{\lambda}{2}-1} \sqrt{\alpha_N^\lambda}. \quad (4.151)$$

Similarly, we get

$$\left\| (\hat{\mu} - \hat{\mu}_1)^{\frac{1}{2}} \hat{\nu} \Phi \right\| \leq N^{-\frac{1}{2}} \sqrt{\alpha_N^\lambda}. \quad (4.152)$$

Since

$$\|U_{1,2} p_1\| \leq N \left(\|v_{\tilde{N}}(\mathbf{x}_1 - \mathbf{x}_2) p_1\| + 2 \|v_{\tilde{N}} * |\phi|^2\|_\infty \right), \quad (4.153)$$

Proposition 4.4.5 and (4.4.5), point (c) yield

$$\begin{aligned}\|U_{1,2}p_1\| &\leq CN \left(\|v_{\tilde{N}}\| \|\phi_\tau\|_\infty + \|v_{\tilde{N}}\|_1 \|\phi_\tau\|_\infty^2 \right) \\ &\leq CN \|\phi_\tau\|_\infty \left(\tilde{N}^{\frac{d\beta}{2}} + \|\phi_\tau\|_\infty \right) \\ &= CN \|\phi_\tau\|_\infty \left(\varepsilon^{-\frac{d}{s+2}} N^{\frac{d\beta}{2}} + \|\phi_\tau\|_\infty \right)\end{aligned}$$

and thus (c) is bounded by

$$C \|\phi_\tau\|_\infty N^{-\frac{1-\lambda}{2}} \alpha_N^\lambda \left(\varepsilon^{-\frac{d}{s+2}} N^{\frac{d\beta}{2}} + \|\phi_\tau\|_\infty \right). \quad (4.154)$$

Conjecture 4.1.3 then implies that (c) is smaller or equal to

$$CN^{-\frac{1-\lambda}{2}} \alpha_N^\lambda \left(1 + \varepsilon^{-\frac{d}{s+2}} N^{\frac{d\beta}{2}} \right). \quad (4.155)$$

□

Proof of Theorem 4.4.2. By Lemma (4.4.7), Proposition (4.4.8) and the condition $\lambda < 1$, we get that

$$\dot{\alpha}_N^\lambda(\Phi_\tau, \varphi_\tau) \leq \left(1 + \varepsilon^{-\frac{3}{s+2}} N^{-\frac{1-\lambda-3\beta}{2}} \right) \alpha_N^\lambda(\Psi_0, \phi_0) + \varepsilon^{-\frac{6}{s+2}} N^{3\beta-\lambda}. \quad (4.156)$$

Grönwall's Lemma then yields

$$\begin{aligned}\alpha_N^\lambda(\Phi_\tau, \varphi_\tau) &\leq \\ &\leq \frac{\varepsilon^{-\frac{6}{s+2}} N^{3\beta-\lambda}}{\left(1 + \varepsilon^{-\frac{3}{s+2}} N^{-\frac{1-\lambda-3\beta}{2}} \right)} \left(e^{\left(1 + \varepsilon^{-\frac{3}{s+2}} N^{-\frac{1-\lambda-3\beta}{2}} \right) \tau} - 1 \right) \\ &\quad + \alpha_N^\lambda(\Phi_0, \phi_0) e^{\left(1 + \varepsilon^{-\frac{3}{s+2}} N^{-\frac{1-\lambda-3\beta}{2}} \right) \tau}, \quad (4.157)\end{aligned}$$

which concludes the proof of the Theorem.

□

4.5 From the Hartree to the Gross-Pitaevskii Equation

We now prove that the solutions to (4.13) and (4.4) remain close at later times, when starting from the same initial datum. This is the content of next Theorem.

Theorem 4.5.1. Assume Conjecture 4.1.3 and let ϕ_0 be such that $\|\phi_0\|_\infty = \mathcal{O}(1)$. Assume also that

$$\mathcal{E}^{\text{GP}}[\phi_0] \leq E^{\text{GP}} + \xi \quad (4.158)$$

for some $\xi \gg \varepsilon |\log \varepsilon|$. Then,

$$\|\phi_\tau - \varphi_\tau\| \leq C \left[\sqrt{\xi} + \frac{\xi}{\tilde{N}^{\frac{\beta}{2}} \varepsilon^2} + \frac{|\log \varepsilon|^{\frac{3}{4}}}{\tilde{N}^{\frac{\beta}{2}} \varepsilon^{\frac{5}{4}}} \right] \tau. \quad (4.159)$$

Proof. We first consider the time derivative of the L^2 -norm squared of the difference between the two solutions. We get

$$\partial_\tau \|\phi_\tau - \varphi_\tau\|^2 = 2\text{Im} \langle \phi_\tau - \varphi_\tau, |\phi_\tau|^2 \phi_\tau - v_{\tilde{N}} * |\varphi_\tau|^2 \varphi_\tau \rangle \quad (4.160)$$

$$= 2\text{Im} \langle \phi_\tau - \varphi_\tau, \left(|\phi_\tau|^2 - v_{\tilde{N}} * |\phi_\tau|^2 \right) \phi_\tau \rangle \quad (4.161)$$

$$+ 2\text{Im} \langle \phi_\tau - \varphi_\tau, \left(v_{\tilde{N}} * |\phi_\tau|^2 - v_{\tilde{N}} * |\varphi_\tau|^2 \right) \phi_\tau \rangle \quad (4.162)$$

$$\leq 2 \|\phi_\tau - \varphi_\tau\| \|\phi_\tau\|_\infty \left(\left\| |\phi_\tau|^2 - v_{\tilde{N}} * |\phi_\tau|^2 \right\| \right) \quad (4.163)$$

$$+ \|v_{\tilde{N}}\|_1 \left\| |\phi_\tau|^2 - |\varphi_\tau|^2 \right\|. \quad (4.164)$$

For the first term, we use that $v_{\tilde{N}}$ tends to a Dirac delta, to get

$$\begin{aligned} \left| |\phi_\tau(\mathbf{x})|^2 - v_{\tilde{N}} * |\phi_\tau|^2(\mathbf{x}) \right| &\leq \\ &\leq \frac{2 \|\phi_\tau\|_\infty}{\tilde{N}^\beta} \int_0^1 ds \int_{\mathbb{R}^3} d\mathbf{y} |\mathbf{y}| v(\mathbf{y}) \left| \nabla \phi_\tau \left(\mathbf{x} - \frac{s\mathbf{y}}{\tilde{N}^\beta} \right) \right|. \end{aligned} \quad (4.165)$$

Hence, we can estimate

$$\left\| |\phi_\tau|^2 - v_{\tilde{N}} * |\phi_\tau|^2 \right\| \leq \frac{2 \|\phi_\tau\|_\infty}{\tilde{N}^\beta} \int_{\mathbb{R}^3} d\mathbf{y} |\mathbf{y}| v(\mathbf{y}) \|\nabla \phi_\tau\| \leq \quad (4.166)$$

$$\leq \frac{C}{\tilde{N}^\beta} \|\nabla \phi_\tau\|. \quad (4.167)$$

On the other hand, by (4.158) and Proposition 4.3.2, we bound the kinetic energy of the state φ_τ as

$$\|\nabla \varphi_\tau\|^2 \leq \frac{C\sqrt{\xi}}{\varepsilon^2} \left(\sqrt{\xi} + \frac{1}{\tilde{N}^\beta \varepsilon} \right). \quad (4.168)$$

Thanks to Conjecture 4.1.3, (4.166), (4.168) and Corollary 4.3.3, we then get

$$\partial_\tau \|\phi_\tau - \varphi_\tau\| \leq \frac{C\xi}{\tilde{N}^{\frac{\beta}{2}} \varepsilon^2} + \frac{C |\log \varepsilon|^{\frac{3}{4}}}{\tilde{N}^{\frac{\beta}{2}} \varepsilon^{\frac{5}{4}}} + C\sqrt{\xi} \quad (4.169)$$

from which the result immediately follows. □

4.6 Proof of Theorem 4.1.5

First notice that the change of length and time scales implies

$$\left\| \gamma_{\Psi_t}^{(1)} - P_{\psi_t} \right\| = \left\| \gamma_{\Phi_\tau}^{(1)} - P_{\phi_\tau} \right\| \leq \left\| \gamma_{\Phi_\tau}^{(1)} - P_{\varphi_\tau} \right\| + \|P_{\varphi_\tau} - P_{\phi_\tau}\| \quad (4.170)$$

$$\leq \left\| \gamma_{\Phi_\tau}^{(1)} - P_{\varphi_\tau} \right\| + 2 \|\varphi_\tau - \phi_\tau\|. \quad (4.171)$$

By (4.14), (4.16) and Corollary 4.4.3, we obtain that, for any fixed time t ,

$$\left\| \gamma_{\Phi_\tau}^{(1)} - P_{\varphi_\tau} \right\| \leq C \varepsilon^{-\frac{6}{s+2}} N^{3\beta-\lambda} e^{C\tau} \left(1 + \varepsilon^{-\frac{6}{s+2}} N^{3\beta-\lambda} e^{C\tau} \right) \quad (4.172)$$

$$= C \varepsilon^{-\frac{6}{s+2}} N^{3\beta-\lambda} e^{C\varepsilon^{-\frac{2(s+3)}{s+2}} t}. \quad (4.173)$$

On the other hand, (4.15) and Theorem 4.5.1 yield

$$\|\varphi_\tau - \phi_\tau\| \leq C \frac{|\log \varepsilon|^{\frac{3}{4}}}{N^\beta \varepsilon^{\frac{5s+2}{4(s+2)}}} \tau \equiv C \frac{|\log \varepsilon|^{\frac{3}{4}}}{N^\beta \varepsilon^{\frac{13}{4}}} t. \quad (4.174)$$

Setting $\delta := 1 - \lambda - 3\beta$, the final result is then proven.