Derivation of the Gross-Pitaevskii Hierarchy

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Abstract

We report on some recent results regarding the dynamical behavior of a trapped Bose-Einstein condensate, in the limit of a large number of particles. These results were obtained in [4], a joint work with L. Erdős and H.-T. Yau.

1 Introduction

In the last years, progress in the experimental techniques has made the study of dilute Bose gas near the ground state a hot topic in physics. For the first time, the existence of Bose-Einstein condensation for trapped gases at very low temperatures has been verified experimentally. The experiments were conducted observing the dynamics of Bose systems, trapped by strong magnetic field and cooled down at very low temperatures, when the confining traps are switched off. It seems therefore important to have a good theoretical description of the dynamics of the condensate. Already in 1961 Gross [7, 8] and Pitaevskii [14] proposed to model the many body effects in a trapped dilute Bose gas by a nonlinear on-site self interaction of a complex order parameter (the condensate wave function u_t). They derived the Gross-Pitaevskii equation

$$i\partial_t u_t = -\Delta u_t + 8\pi a_0 |u_t|^2 u_t \tag{1}$$

for the evolution of u_t. Here a_0 is the scattering length of the pair interaction. A mathematically rigorous justification of this equation is still missing. The aim of this article is to report on recent partial results towards the derivation of (1) starting from the microscopic quantum dynamics in the limit of a large number of particles. Here we only expose the main ideas: for more details, and for all the proofs, we refer to [4].

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Also in the mathematical analysis of dilute bosonic systems some important progress has recently been made. In [13], Lieb and Yngvason give a rigorous proof of a formula for the leading order contribution to the ground state energy of a dilute Bose gas (the correct upper bound for the energy was already obtained by Dyson in [2], for the case of hard spheres). This important result inspired a lot of subsequent works establishing different properties of the ground state of the Bose system. In [12], the authors give a proof of the asymptotic exactness of the Gross-Pitaevskii energy functional for the computation of the ground state energy of a trapped Bose gas. In [10], the complete condensation of the ground state of a trapped Bose gas is proven. For a review of recent results on dilute Bose systems we refer to [11]. All these works investigate the properties of the ground state of the system. Here, on the other hand, we are interested in the dynamical behavior.

Next, we want to describe our main result in some details. To this end, we need to introduce some notation. From now on we consider a system of N bosons trapped in a box $\Lambda \subset \mathbb{R}^3$ with volume one and we impose periodic boundary conditions. In order to describe the interaction among the bosons, we choose a positive, smooth, spherical symmetric potential $V(x)$ with compact support and with scattering length a_0.

Let us briefly recall the definition of the scattering length a_0 of the potential $V(x)$. To define a_0 we consider the radial symmetric solution $f(x)$ of the zero energy one-particle Schrödinger equation

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

with the condition $f(x) \to 1$ for $|x| \to \infty$. Since the potential has compact support, we can define the scattering length a_0 associated to $V(x)$ by the equation $f(x) = 1 - a_0/|x|$ for x outside the support of $V(x)$ (this definition can be generalized by $a_0 = \lim_{r\to\infty} r(1-f(r))$, if V has unbounded support but still decays sufficiently fast at infinity). Another equivalent characterization of the scattering length is given by the formula

$$\int \mathrm{d}x\, V(x) f(x) = 8\pi a_0. \tag{3}$$

Physically, a_0 is a measure of the effective range of the potential $V(x)$.

The Hamiltonian of the N-boson system is then given by

$$H = -\sum_{j=1}^{N} \Delta_j + \sum_{i<j} V_a(x_i - x_j) \tag{4}$$

with $V_a(x) = (a_0/a)^2 V((a_0/a)x)$. By scaling, V_a has scattering length a. In the following we keep a_0 fixed (of order one) and we vary a with N, so that when N tends to infinity a approaches zero. In order for the Gross-Pitaevskii theory to be relevant we have to take a of order N^{-1} (see [12] for a discussion of other possible scalings). In the following we choose therefore $a = a_0/N$, and thus $V_a(x) = N^2 V(Nx)$. Note that, with this choice of a, the Hamiltonian (4) can be viewed as a special case of the mean-field Hamiltonian

$$H_{\text{mf}} = -\sum_{j=1}^{N} \Delta_j + \frac{1}{N} \sum_{i<j} \beta^3 V(\beta(x_i - x_j))\,. \tag{5}$$

The Gross-Pitaevskii scaling is recovered when $\beta = N$. We study the dynamics generated by (5) for other choices of β ($\beta = N^\alpha$, with $\alpha < 3/5$) in [3].

Since we have N particles in a box of volume one, the density is given by $\rho = N$. Hence, the total number of particles interacting at a given time with a fixed particle in the system is typically of order $\rho a^3 \simeq N^{-2} \ll 1$. This means that our system is actually a very dilute gas, scaled so that the total volume remains fixed to one.

The dynamics of the N-boson system is determined by the Schrödinger equation

$$i\partial_t \psi_{N,t} = H\psi_{N,t} \tag{6}$$

for the wave function $\psi_{N,t} \in L^2(\mathbb{R}^{3N}, \mathrm{d}\mathbf{x})$. Instead of describing the quantum mechanical system through its wave-function we can describe it by the corresponding density matrix $\gamma_{N,t} = |\psi_{N,t}\rangle\langle\psi_{N,t}|$ which is the orthogonal projection onto $\psi_{N,t}$. We choose the normalization so that $\operatorname{Tr}\gamma_{N,t} = 1$. The Schrödinger equation (6) takes the form

$$i\partial_t \gamma_{N,t} = [H, \gamma_{N,t}]\,. \tag{7}$$

For large N this equation becomes very difficult to solve, even numerically. Therefore, it is desirable to have an easier description of the dynamics of the system in the limit $N \to \infty$, assuming we are only interested in its macroscopic behavior, resulting from averaging over the N particles. In order to investigate the macroscopic dynamics, we introduce the marginal distributions associated to the density matrix $\gamma_{N,t}$. The k-particle marginal distribution $\gamma^{(k)}_{N,t}$ is defined by taking the partial trace over the last $N-k$ variables. That is, the kernel of $\gamma^{(k)}_{N,t}$ is given by

$$\gamma^{(k)}_{N,t}(\mathbf{x}_k; \mathbf{x}'_k) = \int \mathrm{d}\mathbf{x}_{N-k}\, \gamma_{N,t}(\mathbf{x}_k, \mathbf{x}_{N,k}; \mathbf{x}'_k, \mathbf{x}_{N-k})$$

where $\gamma_{N,t}(\mathbf{x}; \mathbf{x}')$ denotes the kernel of the density matrix $\gamma_{N,t}$. Here and in the following we use the notation $\mathbf{x} = (x_1, \dots, x_N)$, $\mathbf{x}_k = (x_1, \dots, x_k)$, $\mathbf{x}_{N-k} = (x_{k+1}, \dots, x_N)$, and analogously for the primed variables. By definition, the k-particle marginal distributions satisfy the normalization condition

$$\operatorname{Tr}\gamma^{(k)}_{N,t} = 1 \qquad \text{for all} \quad k = 1, \dots, N\,.$$

In contrast to the density matrix $\gamma_{N,t}$, one can expect that, for fixed k, the marginal distribution $\gamma^{(k)}_{N,t}$ has a well defined limit $\gamma^{(k)}_{\infty,t}$ for $N \to \infty$ (with respect to some suitable weak topology), whose dynamics can be investigated. In particular, the Gross-Pitaevskii equation (1) is expected to describe the time evolution of the limit $\gamma^{(1)}_{\infty,t}$ of the one-particle marginal distribution, provided $\gamma^{(1)}_{\infty,t} = |u_t\rangle\langle u_t|$ is a pure state. Eq. (1) can be generalized, for $\gamma^{(1)}_{\infty,t}$ describing a mixed state, to

$$i\partial_t \gamma^{(1)}_{\infty,t}(x;x') = (-\Delta + \Delta')\gamma^{(1)}_{\infty,t}(x;x') + 8\pi a_0 \left(\gamma^{(1)}_{\infty,t}(x;x) - \gamma^{(1)}_{\infty,t}(x';x')\right)\gamma^{(1)}_{\infty,t}(x;x'), \tag{8}$$

which we again denote as the Gross-Pitaevskii equation.

To understand the origin of (8), we start from the dynamics of the marginals $\gamma^{(k)}_{N,t}$, for finite N. From the Schrödinger equation (7), we can easily derive a hierarchy of N equations, commonly called the BBGKY hierarchy, describing the evolution of the distributions $\gamma^{(k)}_{N,t}$, for $k = 1, \ldots, N$:

$$\begin{aligned} i\partial_t \gamma^{(k)}_{N,t}(\mathbf{x}_k;\mathbf{x}'_k) = &\sum_{j=1}^{k}(-\Delta_{x_j} + \Delta_{x'_j})\gamma^{(k)}_{N,t}(\mathbf{x}_k;\mathbf{x}'_k) + \sum_{j\neq\ell}^{k}(V_a(x_j - x_\ell) - V_a(x'_j - x'_\ell))\gamma^{(k)}_{N,t}(\mathbf{x}_k;\mathbf{x}'_k) \\ &+ (N-k)\sum_{j=1}^{k}\int \mathrm{d}x_{k+1}(V_a(x_j - x_{k+1}) - V_a(x'_j - x_{k+1}))\,\gamma^{(k+1)}_{N,t}(\mathbf{x}_k, x_{k+1};\mathbf{x}'_k, x_{k+1}). \end{aligned} \tag{9}$$

Here we use the convention that $\gamma^{(k)}_{N,t} = 0$, for $k > N$. Hence, the one-particle marginal density $\gamma^{(1)}_{N,t}$ satisfies

$$\begin{aligned} i\partial_t \gamma^{(1)}_{N,t}(x_1;x'_1) = &(-\Delta_{x_1} + \Delta_{x'_1})\gamma^{(1)}_{N,t}(x_1;x'_1) \\ &+ (N-1)\int \mathrm{d}x_2\,\left(V_a(x_1 - x_2) - V_a(x'_1 - x_2)\right)\gamma^{(2)}_{N,t}(x_1, x_2;x'_1, x_2)\,. \end{aligned} \tag{10}$$

In order to get a closed equation for $\gamma^{(1)}_{N,t}$ we need to assume some relation between $\gamma^{(1)}_{N,t}$ and $\gamma^{(2)}_{N,t}$. The most natural assumption consists in taking the two particle marginal to be the product of two identical copies of the one particle marginal. Although this kind of factorization cannot be true for finite N, it may hold in the limit $N \to \infty$. We suppose therefore that $\gamma^{(k)}_{\infty,t}$, for $k = 1, 2$, is a limit point of $\gamma^{(k)}_{N,t}$, with respect to some weak topology, with the factorization property

$$\gamma^{(2)}_{\infty,t}(x_1, x_2;x'_1, x'_2) = \gamma^{(1)}_{\infty,t}(x_1;x'_1)\gamma^{(1)}_{\infty,t}(x_2;x'_2)\,.$$

Under this assumption we could naively guess that, in the limit $N \to \infty$, Eq. (10) takes the form

$$i\partial_t \gamma^{(1)}_{\infty,t}(x_1;x'_1) = (-\Delta_{x_1} + \Delta_{x'_1})\gamma^{(1)}_{\infty,t}(x_1;x'_1) + \left(Q_t(x_1) - Q_t(x'_1)\right)\gamma^{(1)}_{\infty,t}(x_1;x'_1) \tag{11}$$

with

$$\begin{aligned} Q_t(x_1) &= \lim_{N\to\infty} N\int \mathrm{d}x_2\, V_a(x_1 - x_2)\gamma^{(1)}_{\infty,t}(x_2;x_2) \\ &= \lim_{N\to\infty}\int \mathrm{d}x_2\, N^3 V(N(x_1 - x_2))\gamma^{(1)}_{\infty,t}(x_2;x_2) \\ &= b_0\gamma^{(1)}_{\infty,t}(x_1;x_1) \end{aligned}$$

where we defined $b_0 = \int \mathrm{d}x\, V(x)$. Using the last equation, (11) can be rewritten as

$$i\partial_t \gamma^{(1)}_{\infty,t}(x_1;x_1') = (-\Delta_{x_1} + \Delta_{x_1'})\gamma^{(1)}_{\infty,t}(x_1;x_1') + b_0 \left(\gamma^{(1)}_{\infty,t}(x_1;x_1) - \gamma^{(1)}_{\infty,t}(x_1';x_1')\right) \gamma^{(1)}_{\infty,t}(x_1;x_1') \tag{12}$$

which is exactly the Gross-Pitaevskii equation (8), but with the wrong coupling constant in front of the non-linear term (b_0 instead of $8\pi a_0$). The fact that we get the wrong coupling constant suggests that something was not completely correct with the naif argument leading from (10) to (12). Reconsidering the argument, the origin of the error is quite clear: when passing to the limit $N \to \infty$ we first replaced $\gamma^{(2)}_{N,t}$ with $\gamma^{(2)}_{\infty,t}$ and only after this replacement we took the limit $N \to \infty$ in the potential. This procedure gives the wrong result because the marginal distribution $\gamma^{(2)}_{N,t}$ has a short scale structure living on the scale $1/N$, which is the same length scale characterizing the potential $V_a(x)$. The short scale structure of $\gamma^{(2)}_{N,t}$ (which describes the correlations among the particles) disappears when the weak limit is taken, so that $\gamma^{(2)}_{\infty,t}$ lives on a length scale of order one. Therefore, in (12) we get the wrong coupling constant because we erroneously disregarded the effect of the correlations present in $\gamma^{(2)}_{N,t}$. It is hence clear that in order to derive the Gross-Pitaevskii equation (8) with the correct coupling constant $8\pi a_0$, we need to take into account the short scale structure of $\gamma^{(2)}_{N,t}$. To this end we begin by studying the ground state of the system.

A good approximation for the ground state wave function of the N boson system is given by

$$W(\mathbf{x}) = \prod_{i<j}^{N} f(N(x_i - x_j))$$

where $f(x)$ is defined by (2) (then $f(Nx)$ solves the same equation (2) with V replaced by V_a). Since we assumed the potential to be compactly supported (let R denote the radius of its support), we have $f(x) = 1 - a_0/|x|$, for $|x| > R$, and thus $f(Nx) = 1 - a_0/N|x| = 1 - a/|x|$, for $|x| > Ra$. A similar ansatz for the ground state wave function was already used by Dyson in [2] to prove his upper bound on the ground state energy. In order to describe states of the condensate, it seems appropriate to consider wave functions of the form

$$\psi_N(\mathbf{x}) = W(\mathbf{x})\phi_N(\mathbf{x})$$

where $\phi_N(\mathbf{x})$ varies over distances of order one, and is approximately factorized, that is $\phi_N(\mathbf{x}) \simeq \prod_{j=1}^N \phi(x_j)$. Assuming for the moment that this form is preserved under the time-evolution we have

$$\gamma^{(2)}_{N,t}(x_1,x_2;x_1',x_2') \simeq f(N(x_1-x_2))f(N(x_1'-x_2'))\gamma^{(1)}_{N,t}(x_1;x_1')\gamma^{(1)}_{N,t}(x_2;x_2')\,.$$

Thus, for finite N, $\gamma^{(2)}_{N,t}$ is not exactly factorized and has a short scale structure given by the function $f(Nx)$. When we consider the limit $N \to \infty$ of the second term on the right hand side of (10) we obtain

$$
\begin{aligned}
&\lim_{N\to\infty} N\int \mathrm{d}x_2\, V_a(x_1-x_2)\gamma^{(2)}_{N,t}(x_1,x_2;x_1',x_2) \\
&\qquad\qquad = \lim_{N\to\infty} N^3\int \mathrm{d}x_2\, V(N(x_1-x_2))f(N(x_1-x_2))\gamma^{(1)}_{\infty,t}(x_1;x_1')\gamma^{(1)}_{\infty,t}(x_2;x_2) \\
&\qquad\qquad = 8\pi a_0\gamma^{(1)}_{\infty,t}(x_1;x_1')\gamma^{(1)}_{\infty,t}(x_1;x_1)
\end{aligned}
\tag{13}
$$

where we used Eq. (3) and the fact that $\gamma^{(1)}_{N,t}$ lives on a scale of order one (and thus we can replace it by $\gamma^{(1)}_{\infty,t}$ without worrying about the correlations). This leads to the Gross-Pitaevskii equation for $\gamma^{(1)}_{\infty,t}$,

$$
i\partial_t\gamma^{(1)}_{\infty,t}(x_1;x_1') = \left(-\Delta_{x_1}+\Delta_{x_1'}\right)\gamma^{(1)}_{\infty,t}(x_1;x_1') + 8\pi a_0\left(\gamma^{(1)}_{\infty,t}(x_1;x_1)-\gamma^{(1)}_{\infty,t}(x_1';x_1')\right)\gamma^{(1)}_{\infty,t}(x_1;x_1')
$$

which has the correct coupling constant in front of the non-linear term.

Note that the factorization

$$
\gamma^{(2)}_{\infty,t}(x_1,x_2;x_1',x_2') = \gamma^{(1)}_{\infty,t}(x_1;x_1')\gamma^{(1)}_{\infty,t}(x_2;x_2')
$$

still holds true, because the short scale structure of $\gamma^{(2)}_{N,t}$ vanishes when the weak limit $N\to\infty$ is taken. The short scale structure only shows up in the Gross-Pitaevskii equation due to the singularity of the potential.

In order to make this heuristic argument for the derivation of the Gross-Pitaevskii equation rigorous, we are faced with two major steps.

i) In the first step we have to prove that the k-particle marginal density in the limit $N\to\infty$ really has the short scale structure we discussed above. That is we have to prove that, for large N,

$$
\gamma^{(k+1)}_{N,t}(\mathbf{x}_{k+1};\mathbf{x}'_{k+1}) \simeq \left(\prod_{i<j}^{k+1} f(N(x_i-x_j))f(N(x_i'-x_j'))\right)\gamma^{(k+1)}_{\infty,t}(\mathbf{x}_{k+1};\mathbf{x}'_{k+1}) \tag{14}
$$

where $\gamma^{(k+1)}_{\infty,t}$ is the limit of $\gamma^{(k+1)}_{N,t}$ with respect to some suitable weak topology (in the heuristic argument above we considered the case $k=1$, here k is an arbitrary fixed integer $k\geq 1$). Eq. (14) would then imply that, as $N\to\infty$, the last term on the r.h.s. of the BBGKY hierarchy (9) converges to

$$
\lim_{N\to\infty} N\int \mathrm{d}x_{k+1}\, V_a(x_j-x_{k+1})\gamma^{(k+1)}_{N,t}(\mathbf{x}_{k+1};\mathbf{x}'_{k+1}) = 8\pi a_0\gamma^{(k+1)}_{\infty,t}(\mathbf{x}_k,x_j;\mathbf{x}'_k,x_j)\,.
$$

Therefore, if we could also prove that the second term on the r.h.s. of (9) vanishes in the limit $N \to \infty$ (as expected, because formally of the order N^{-1}), then it would follow that the family $\gamma^{(k)}_{\infty,t}$ satisfies the Gross-Pitaevskii hierarchy

$$\begin{aligned} i\partial_t \gamma^{(k)}_{\infty,t}(\mathbf{x}_k;\mathbf{x}'_k) &= \sum_{j=1}^k \left(-\Delta_j + \Delta'_j\right) \gamma^{(k)}_{\infty,t}(\mathbf{x}_k;\mathbf{x}'_k) \\ &\quad + 8\pi a_0 \sum_{j=1}^k \int \mathrm{d}x_{k+1} \, \left(\delta(x_{k+1}-x_j) - \delta(x_{k+1}-x'_j)\right) \gamma^{(k+1)}_{\infty,t}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1}) \end{aligned} \tag{15}$$

for all $k \geq 1$. We already know that this infinite hierarchy of equation has a solution. In fact the factorized family of densities $\gamma^{(k)}_{\infty,t}(\mathbf{x}_k;\mathbf{x}'_k) = \prod_{j=1}^k \gamma^{(1)}_{\infty,t}(x_j;x'_j)$ is a solution of (15) if and only if $\gamma^{(1)}_{\infty,t}$ solves the Gross-Pitaevskii equation (8).

ii) Secondly, we need to prove that the densities $\gamma^{(k)}_{\infty,t}$ factorize, that is, that, for all $k \geq 1$,

$$\gamma^{(k)}_{\infty,t}(\mathbf{x}_k;\mathbf{x}'_k) = \prod_{j=1}^k \gamma^{(1)}_{\infty,t}(x_j;x'_j)\,. \tag{16}$$

Then, from (15) and (16), it would follow that $\gamma^{(1)}_{\infty,t}$ is a solution of the Gross-Pitaevskii equation (8). Note that, since we already know that (15) has a factorized solution, in order to prove (16) it is enough to prove the uniqueness of the solution of the infinite hierarchy (15).

Unfortunately, due to the singularity of the δ-function, we are still unable to prove that (15) has a unique solution and thus we cannot prove part ii) (the best result in this direction is the proof of the uniqueness for the hierarchy with a Coulomb singularity, see [5]). On the other hand we can complete part i) of our program, that is, we can prove that any limit point $\{\gamma^{(k)}_{\infty,t}\}_{k\geq 1}$ of the family $\{\gamma^{(k)}_{N,t}\}_{k=1}^N$ (with respect to an appropriate weak topology), satisfies the infinite hierarchy (15), provided we replace the original Hamiltonian H with a slightly modified version $\widetilde{H}$, where we artificially modify the interaction when a large number of particles come into a region with diameter much smaller than the typical inter-particle distance. Since H agrees with $\widetilde{H}$, apart in the very rare event (rare with respect to the expected typical distribution of the particles) that many particles come very close together, we don't expect this modification to change the macroscopic dynamics of the system: but unfortunately we cannot control this effect rigorously.

Note that the Gross-Pitaevskii equation (1) is a nonlinear Hartree equation

$$i\partial_t u_t = -\Delta u_t + (V * |u_t|^2) u_t \tag{17}$$

in the special case $V(x) = 8\pi a_0 \delta(x)$. In the literature there are several works devoted to the derivation of (17) from the N-body Schrödinger equation. The first results were obtained by Hepp in [9], for a smooth potential $V(x)$, and by Spohn in [15], for bounded $V(x)$. Later, Ginibre and Velo extended these results to singular potentials in [6]: their result is limited to coherent initial states, for which the number of particles cannot be fixed. In [5], Erdős and Yau derived (17) for the Coulomb potential $V(x) = \pm 1/|x|$. More recently, Adami, Bardos, Golse and Teta obtained partial results for the potential $V(x) = \delta(x)$, which leads to the Gross-Pitaevskii equation, in the case of one-dimensional systems; see [1].

2 The Main Result

In this section we explain how we need to modify the Hamiltonian and then we state our main theorem. In order to derive (15) it is very important to find a good approximation for the wave function of the ground state of the N boson system. We need an approximation which reproduces the correct short scale structure and, at the same time, does not become too singular (so that error terms can be controlled). Our first guess

$$W(\mathbf{x}) = \prod_{i<j} f_a(x_i - x_j) = \prod_{i<j} f(N(x_i - x_j)) \tag{18}$$

is unfortunately not good enough. First of all we need to cutoff the correlations at large distances (we want $f_a(x) = 1$ for $|x| \gg a$). To this end we fix a length scale $\ell_1 \gg a$, and we consider the Neumann problem on the ball $\{x : |x| \le \ell_1\}$ (we will choose $\ell_1 = N^{-2/3+\kappa}$ for a small $\kappa > 0$). We are interested in the solution of the ground state problem

$$(-\Delta + 1/2 V_a(x))(1 - w(x)) = e_{\ell_1}(1 - w(x))$$

on $\{x : |x| \le \ell_1\}$, with the normalization condition $w(x) = 0$ for $|x| = \ell_1$. Here e_{ℓ_1} is the lowest possible eigenvalue. It is easy to check that, up to contributions of lower order, $e_{\ell_1} \simeq 3a/\ell_1^3$. We can extend $w(x)$ to be identically zero, for $|x| \ge \ell_1$. Then

$$\begin{aligned}(-\Delta + 1/2 V_a(x))(1 - w(x)) &= q(x)(1 - w(x)), \quad \text{with} \\ q(x) &\simeq \frac{3a}{\ell_1^3}\chi(|x| \le \ell_1)\,.\end{aligned} \tag{19}$$

For $a \ll |x| \ll \ell_1$, the function $1 - w(x)$ still looks very much like $1 - a/|x|$, but now it equals one, for $|x| \ge \ell_1$. Replacing $f_a(x_i - x_j)$ by $1 - w(x_i - x_j)$ in (18) is still not sufficient for our purposes. The problem is that the wave function $\prod_{i<j}(1 - w(x_i - x_j))$ becomes very singular when a large number of particles come very close together. We introduce another cutoff to avoid this problem. We fix a new length scale $\ell \gg \ell_1 \gg a$, such that $\ell \ll N^{-1/3}$ (that is ℓ is still much smaller than the typical inter-particle distance: we will choose $\ell = N^{-2/5-\kappa}$ for a small $\kappa > 0$). Then, for fixed indices i and j, and for an arbitrary fixed number $K \ge 1$, we cutoff the correlation between particles i and j (that is we replace $1 - w(x_i - x_j)$ by one) whenever at least K other particles come inside a ball of radius ℓ around i and j. In order to keep our exposition as clear as possible we choose $K = 1$, that is we cutoff correlations if at least three particles come very close together. But there is nothing special about $K = 1$: what we really need to avoid are correlations among a macroscopic number of particles, all very close together. To implement our cutoff we introduce, for fixed indices i, j, a function $F_{ij}(\mathbf{x})$ with the property that

$$\begin{aligned} F_{ij}(\mathbf{x}) &\cong 1 \quad \text{if} \quad \begin{cases} |x_i - x_m| & \gg \ell \\ |x_j - x_m| & \gg \ell \end{cases} \qquad \text{for all } m \neq i, j \\ F_{ij}(\mathbf{x}) &\cong 0 \quad \text{otherwise.} \end{aligned}$$

Instead of using the wave function $\prod_{i<j}(1 - w(x_i - x_j))$ we will approximate the ground state of the N boson system by

$$W(\mathbf{x}) = \prod_{i<j} (1 - w(x_i - x_j) F_{ij}(\mathbf{x})) \tag{20}$$

(the exact definition of $W(\mathbf{x})$ is a little bit more complicated; see [4], Section 2.3). The introduction of the cutoffs F_{ij} in the wave function $W(\mathbf{x})$ forces us to modify the Hamiltonian H. To understand how H has to be modified, we compute its action on $W(\mathbf{x})$. We have, using (19),

$$\begin{aligned} W(\mathbf{x})^{-1}(HW)(\mathbf{x}) = &\sum_{i,j} q(x_i - x_j) \\ &+ \sum_{i,j} \left((1/2)V_a(x_i - x_j) - q(x_i - x_j)\right)(1 - F_{ij}(\mathbf{x})) \\ &+ \text{lower order contributions.} \end{aligned}$$

The "lower order contributions" are terms containing derivatives of F_{ij}: they need some control, but they are not very dangerous for our analysis. On the other hand, the second term on the r.h.s. of the last equation, whose presence is due to the introduction of the cutoffs F_{ij}, still contains the potential V_a and unfortunately we cannot control it with our techniques. Therefore, we artificially remove it, defining a new Hamiltonian $\widetilde{H}$, by

$$\widetilde{H} = H - \sum_{i,j} \left((1/2)V_a(x_i - x_j) - q(x_i - x_j)\right)(1 - F_{ij}(\mathbf{x})) \, .$$

Note that the new Hamiltonian $\widetilde{H}$ equals the physical Hamiltonian H unless three or more particles come at distances less than $\ell \ll N^{-1/3}$. This is a rare event, and thus we don't expect the modification of the Hamiltonian H to change in a macroscopic relevant way the dynamics of the system.

Before stating our main theorem, we still have to specify the topology we use in taking the limit $N \to \infty$ of the marginal distributions $\gamma^{(k)}_{N,t}$. It is easy to check that, for every $k \geq 1$, $\gamma^{(k)}_{N,t}(\mathbf{x}_k; \mathbf{x}'_k) \in$

$L^2(\Lambda^k \times \Lambda^k)$. This motivates the following definition. For $\Gamma = \{\gamma^{(k)}\}_{k\geq 1} \in \bigoplus_{k\geq 1} L^2(\Lambda^k \times \Lambda^k)$, and for a fixed $\nu > 1$, we define the two norms

$$\|\Gamma\|_- := \sum_{k\geq 0} \nu^{-k} \|\gamma^{(k)}\|_2 \qquad \text{and} \qquad \|\Gamma\|_+ := \sup_{k\geq 1} \nu^k \|\gamma^{(k)}\|_2 \tag{21}$$

where $\|.\|_2$ denotes the L^2-norm on $\Lambda^k \times \Lambda^k$. We have to introduce the parameter $\nu > 1$ to make sure that, for $\Gamma_{N,t} = \{\gamma^{(k)}_{N,t}\}_{k=1}^N$, the norm $\|\Gamma_{N,t}\|_-$ is finite (choosing ν large enough, we find $\|\Gamma_{N,t}\|_- \leq 1$, uniformly in N and t). We also define the Banach spaces

$$\mathcal{H}_- := \{\Gamma = \{\gamma^{(k)}\}_{k\geq 0} \in \bigoplus_{k\geq 1} L^2(\Lambda^k \times \Lambda^k) : \|\Gamma\|_- < \infty\}$$

and

$$\mathcal{H}_+ := \{\Gamma = \{\gamma^{(k)}\}_{k\geq 0} \in \bigoplus_{k\geq 1} L^2(\Lambda^k \times \Lambda^k) : \lim_{k\to\infty} \nu^k \|\gamma^{(k)}\|_2 = 0\}\,.$$

Then we have $(\mathcal{H}_-, \|.\|_-) = (\mathcal{H}_+, \|.\|_+)^*$. This induces a weak* topology on $\mathcal{H}_-$, with respect to which the unit ball $\mathcal{B}_-$ of $\mathcal{H}_-$ is compact (Banach-Alaouglu Theorem). Since the space $\mathcal{H}_+$ is separable, the weak* topology on the unit ball $\mathcal{B}_-$ is metrizable: we can find a metric ρ on $\mathcal{H}_-$, such that a sequence $\Gamma_n \in \mathcal{B}_-$ converges with respect to the weak* topology if and only if it converges with respect to the metric ρ. For a fixed time T, we will also consider the space $C([0,T], \mathcal{B}_-)$ of functions of $t \in [0,T]$, with values in the unit ball $\mathcal{B}_- \subset \mathcal{H}_-$, which are continuous with respect to the metric ρ (or equivalently with respect to the weak* topology of $\mathcal{H}_-$). We equip $C([0,T], \mathcal{B}_-)$ with the metric

$$\widetilde{\rho}(\Gamma_1(t), \Gamma_2(t)) = \sup_{t\in[0,T]} \rho(\Gamma_1(t), \widetilde{\Gamma}_2(t))\,.$$

In the following we will consider the families $\Gamma_{N,t} = \{\gamma^{(k)}_{N,t}\}_{k=1}^N$ as elements of $C([0,T], \mathcal{B}_-)$, and we will study their convergence and their limit points with respect to the metric $\widetilde{\rho}$. We are now ready to state our main theorem.

Theorem 2.1. *Assume $a = a_0/N$, $\ell_1 = N^{-2/3+\kappa}$, $\ell = N^{-2/5-\kappa}$, for some sufficiently small $\kappa > 0$. Assume*

$$(\psi_{N,0}, \widetilde{H}^2 \psi_{N,0}) \leq CN^2\,,$$

where $(.,.)$ denotes the inner product on $L^2(\mathbb{R}^{3N}, \mathrm{d}\mathbf{x})$. Let $\psi_{N,t}$, for $t \in [0,T]$, be the solution of the Schrödinger equation

$$i\partial_t \psi_{N,t} = \widetilde{H} \psi_{N,t} \tag{22}$$

with initial data $\psi_{N,0}$. Then, if $\alpha = (\|V\|_1 + \|V\|_\infty)$ is small enough (of order one) and $\nu > 1$ is large enough (recall that ν enters the definition of the norms (21)), we have:

i) $\Gamma_{N,t} = \{\gamma^{(k)}_{N,t}\}_{k=1}^N$ has at least one (non-trivial) limit point $\Gamma_{\infty,t} = \{\gamma^{(k)}_{\infty,t}\}_{k\geq 1} \in C([0,T], \mathcal{B}_-)$ with respect to the metric $\widetilde{\rho}$.

ii) For any limit point $\Gamma_{\infty,t} = \{\gamma^{(k)}_{\infty,t}\}_{k\geq 1}$ and for all $k \geq 1$, there exists a constant C such that

$$Tr(1-\Delta_i)(1-\Delta_j)\gamma^{(k)}_{\infty,t} \leq C \tag{23}$$

for all $i \neq j$, $t \in [0,T]$.

iii) Any limit point $\Gamma_{\infty,t}$ satisfies the infinite Gross-Pitaevskii hierarchy (15) when tested against a regular function $J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)$:

$$\begin{aligned} \langle J^{(k)}, \gamma^{(k)}_{\infty,t}\rangle = \langle J^{(k)}, \gamma^{(k)}_{\infty,0}\rangle &- i\sum_{j=1}^k \int_0^t \mathrm{d}s \langle J^{(k)}, (-\Delta_j + \Delta'_j)\gamma^{(k)}_{\infty,s}\rangle \\ &- 8i\pi a_0 \sum_{j=1}^k \int_0^t \mathrm{d}s \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \, J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k) \\ &\times \int \mathrm{d}x_{k+1} \left(\delta(x_j - x_{k+1}) - \delta(x'_j - x_{k+1})\right) \gamma^{(k+1)}_{\infty,s}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1}) \,. \end{aligned} \tag{24}$$

Here we use the notation $\langle J^{(k)}, \gamma^{(k)}\rangle = \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \, \overline{J^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)}\, \gamma^{(k)}(\mathbf{x}_k;\mathbf{x}'_k)$.

Remarks.

i) The main assumption of the theorem is the requirement that the expectation of $\widetilde{H}^2$ at $t=0$ is of order N^2. One can prove that this condition is satisfied for $\psi_{N,0}(\mathbf{x}) = W(\mathbf{x})\phi_N(\mathbf{x})$ and ϕ_N sufficiently smooth (see [4], Lemma D1). Physically, this assumption guarantees that the initial wave function $\psi_{N,0}(\mathbf{x})$ has the short-scale structure characteristic of $W(\mathbf{x})$ and, hence, that it describes, locally, a condensate.

ii) It is a priori not clear that the action of the delta-functions in the Gross-Pitaevskii hierarchy (24) is well defined. This fact follows by the bound (23), which makes sure that $\gamma^{(k)}_{\infty,t}$ is sufficiently smooth.

iii) We also need to assume that $\alpha = (\|V\|_\infty + \|V\|_1)$ is small enough (but still of order one). This technical assumption is needed in the proof of the energy estimate, Proposition 3.1.

3 Sketch of the Proof

In this section we explain some of the main ideas used in the proof of Theorem 2.1. Let $\psi_{N,t}$ be the solution of the Schrödinger equation (22) (with the modified Hamiltonian $\widetilde{H}$). We can decompose $\psi_{N,t}$ as

$$\psi_{N,t}(\mathbf{x}) = W(\mathbf{x})\phi_{N,t}(\mathbf{x}),$$

where $W(\mathbf{x})$ is the approximation for the ground state wave function defined in (20). This decomposition is always possible because $W(\mathbf{x})$ is strictly positive.

The main tool in the proof of Theorem 2.1 is an estimate for the L^2-norm of the second derivatives of $\phi_{N,t}$. This bound follows from the following *energy estimate*.

Proposition 3.1. *Assume $a = a_0/N$, $\ell_1 = N^{-2/3+\kappa}$ and $\ell = N^{-2/5-\kappa}$ for $\kappa > 0$ small enough, and suppose $\alpha = (\|V\|_1 + \|V\|_\infty)$ is sufficiently small. Then there exists a constant $C > 0$ such that*

$$\int \mathrm{d}\mathbf{x}\, |(\tilde{H} W \phi)(\mathbf{x})|^2 \geq (C - o(1)) \sum_{i,j=1}^N \int \mathrm{d}\mathbf{x}\, W^2(\mathbf{x}) |\nabla_i \nabla_j \phi(\mathbf{x})|^2 \\ - o(1) \left(N \sum_{i=1}^N \int \mathrm{d}\mathbf{x}\, W^2(\mathbf{x}) |\nabla_i \phi(\mathbf{x})|^2 + N^2 \int \mathrm{d}\mathbf{x}\, W^2(\mathbf{x}) |\phi(\mathbf{x})|^2 \right),$$

where $o(1) \to 0$ as $N \to \infty$.

Remark. The proof of this proposition is the main technical difficulty in our analysis. It is in order to prove this proposition that we need to introduce the cutoffs F_{ij} in the approximate ground state wave function $W(\mathbf{x})$, and that we need to modify the Hamiltonian.

Using the assumption that, at $t = 0$, $(\psi_{N,0}, \widetilde{H}^2 \psi_{N,0}) \leq CN^2$, the conservation of the energy, and the symmetry with respect to permutations, we immediately get the following corollary.

Corollary 3.2. *Suppose the assumptions of Proposition 3.1 are satisfied. Suppose moreover that the initial data $\psi_{N,0}$ is symmetric with respect to permutations and $(\psi_{N,0}, \widetilde{H}^2 \psi_{N,0}) \leq CN^2$. Then there exists a constant C such that*

$$\int W^2(\mathbf{x}) |\nabla_i \nabla_j \phi_{N,t}(\mathbf{x})|^2 \leq C \tag{25}$$

for all $i \neq j$, t and all N large enough.

Remark. The bound (25) is not an estimate for the derivatives of the whole wave function $\psi_{N,t}$. The inequality

$$\int \mathrm{d}\mathbf{x}\, |\nabla_i \nabla_j \psi(\mathbf{x})|^2 < C \tag{26}$$

is wrong, if ψ satisfies $(\psi, \widetilde{H}^2 \psi) \leq CN^2$. In fact, in order for $(\psi, \widetilde{H}^2 \psi)$ to be of order N^2, the wave function $\psi(\mathbf{x})$ needs to have the short scale structure characterizing $W(\mathbf{x})$. This makes (26) impossible to hold true uniformly in N. Only after the singular part $W(\mathbf{x})$ has been factorized out, we can prove bounds like (25) for the derivatives of the remainder. One of the consequences of our energy estimate, and one of the possible interpretation of our result, is that the separation between the singular part of the wave function (living on the scale $1/N$) and its regular part is preserved by the time evolution.

Next we show how the important bound (25) can be used to prove Theorem 2.1. According to the decomposition $\psi_{N,t}(\mathbf{x}) = W(\mathbf{x})\phi_{N,t}(\mathbf{x})$, we define, for $k = 1, \dots, N$, the densities $U^{(k)}_{N,t}(\mathbf{x}_k; \mathbf{x}'_k)$, for $k = 1, \dots, N$, to be, roughly, the k-particle marginal density corresponding to the wave function $\phi_{N,t}$ (the exact definition is a little bit more involved, see [4], Section 4). The estimate (25) for the second derivatives of $\phi_{N,t}$ translates into a bound for the densities $U^{(k)}_{N,t}$:

$$\mathrm{Tr}\,(1-\Delta_i)(1-\Delta_j)U^{(k)}_{N,t} \leq C \tag{27}$$

for all $i, j \leq N$ with $i \neq j$, for all t and for all N large enough.

Moreover, we can show that, for $\nu > 1$ large enough (recall that the parameter ν enters the definition of the norms (21)), the families $U_{N,t} = \{U^{(k)}_{N,t}\}_{k=1}^N$ define an equicontinuous sequence in the space $C([0,T], \mathcal{B}_-)$ (this follows from a careful analysis of the BBGKY hierarchy associated to the Schrödinger equation (22); see [4], Sections 9.1 and 9.2 for more details). Applying standard results (Arzela-Ascoli Theorem), it follows that the sequence $U_{N,t}$ has at least one limit point, denoted $U_{\infty,t} = \{U^{(k)}_{\infty,t}\}_{k\geq 1}$, in the space $C([0,T], \mathcal{B}_-)$. The bound (27) can then be passed to the limit $N \to \infty$, and we obtain

$$\mathrm{Tr}\,(1-\Delta_i)(1-\Delta_j)U^{(k)}_{\infty,t} \leq C$$

for all $i \neq j$ and $t \in [0,T]$.

Next we go back to the family $\Gamma_{N,t} = \{\gamma^{(k)}_{N,t}\}_{k=1}^N$. Clearly, the densities $\gamma^{(k)}_{N,t}$ do not satisfy the estimate (27). In fact, $\gamma^{(k)}_{N,t}$ still contains the short scale structure of $W(\mathbf{x})$ (which, on the contrary, has been factorized out from $U^{(k)}_{N,t}$), and thus cannot have the smoothness required by (27).

It is nevertheless clear that the short scale structure of $\Gamma_{N,t}$ disappears when we consider the limit $N \to \infty$ (in the weak sense specified by Theorem 2.1). In fact, one can prove the convergence of an appropriate subsequence of $\Gamma_{N,t}$ to the limit point $U_{\infty,t}$ of $U_{N,t}$. In other words one can show that limit points of $\Gamma_{N,t}$, denoted by $\Gamma_{\infty,t}$, coincide with the limit points of $U_{N,t}$. Therefore, even though $\Gamma_{N,t}$, for finite N, does not satisfies the bound (27), its limit points $\Gamma_{\infty,t} = \{\gamma^{(k)}_{\infty,t}\}_{k\geq 1}$ do. For every $k \geq 1$ we have

$$\mathrm{Tr}\,(1-\Delta_i)(1-\Delta_j)\gamma^{(k)}_{\infty,t} \leq C \tag{28}$$

for all $i \neq j$ and $t \in [0,T]$. This proves part i) and ii) of Theorem 2.1 (the non-triviality of the limit follows by showing that $\mathrm{Tr}\,\gamma^{(1)}_{\infty,t} = 1$). The bound (28) can then be used to prove part iii) of Theorem 2.1, that is to prove that the family $\Gamma_{\infty,t}$ satisfies the infinite Gross-Pitaevskii hierarchy (24). In fact, having control over the derivatives of $\gamma^{(k)}_{\infty,t}$ allows us to prove the convergence of the potential to a delta-function (that is, it allows us to make (13) rigorous). To this end we use the following lemma (see [4], Section 8).

Lemma 3.3. *Suppose $\delta_\beta(x) = \beta^{-3}h(x/\beta)$, for some regular function h, with $\int h(x) = 1$. Then, for* *any* $1 \leq j \leq k$*, and for any regular function* $J(\mathbf{x}_k;\mathbf{x}'_k)$*, we have*

$$\Big| \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \mathrm{d}x_{k+1}\, J(\mathbf{x}_k;\mathbf{x}'_k)(\delta_\beta(x_j - x_{k+1}) - \delta(x_j - x_{k+1}))\gamma^{(k+1)}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1})\Big| \\ \leq C_J \sqrt{\beta}\, Tr(1-\Delta_j)(1-\Delta_{k+1})\gamma^{(k+1)} \,.$$

Part iii) of Theorem 2.1 can then be proven combining this lemma with the estimates (27) and (28) (see [4], Section 9.4, for more details).

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