Derivation of the time dependent Gross-Pitaevskii equation without positivity condition on the interaction

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May 30, 2018

Abstract

Using a new method [6] it is possible to derive mean field equations from the microscopic N body Schrödinger evolution of interacting particles without using BBGKY hierarchies.

In this paper we wish to analyze scalings which lead to the Gross-Pitaevskii equation which is usually derived assuming positivity of the interaction [1, 2]. The new method for dealing with mean field limits presented in [6] allows us to relax this condition. The price we have to pay for this relaxation is however that we have to restrict the scaling behavior to $\beta < 1/3$ and that we have to assume fast convergence of the reduced one particle marginal density matrix of the initial wave function μ^{Ψ_0} to a pure state $|\varphi_0\rangle\langle\varphi_0|$.

1 Introduction

We are interested in solutions of the N-particle Schrödinger equation

$$i\dot{\Psi}_N^t = H_N \Psi_N^t \tag{1}$$

with symmetric Ψ_N^0 we shall specify below and the Hamiltonian

$$H_N = -\sum_{j=1}^{N} \Delta_j + \sum_{1\le j<k\le N} v_N^\beta(x_j - x_k) + \sum_{j=1}^{N} A^t(x_j) \tag{2}$$

acting on the Hilbert space $L^2(\mathbb{R}^{3N} \to \mathbb{C})$. $\beta \in \mathbb{R}$ stands for the scaling behavior of the interaction. The v_N^β we wish to analyze scale with the particle number in such a way that the interaction energy per particle is of order one. We choose an interaction which is given by

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Assumption 1.1.
$$v_N^\beta(x) = N^{-1+3\beta} v(N^\beta x)$$
with compactly supported, spherically symmetric $v \in L^\infty$.

The trap potential A^t does not depend on N. H_N conserves symmetry, i.e. any symmetric function Ψ_N^0 evolves into a symmetric function Ψ_N^t.

Assume that the initial wave functions $\Psi_N^0 \approx \prod_{j=1}^N \varphi^t(x_j)$ where $\varphi^0 \in L^2$ and that the Gross-Pitaevskii equation

$$i\dot{\varphi}^t = -\left(\Delta + A^t + a|\varphi^t|^2\right)\varphi^t \tag{3}$$

with $a = \int v(x) d^3x$ has a solution. We shall show that also $\Psi_N^t \approx \prod_{j=1}^N \varphi^t(x_j)$ as $N \to \infty$.

The focus of this paper is on interactions which need not be positive. The price we have to pay is that we have to assume comparably fast convergence of the reduced one particle marginal density matrix of the initial wave function μ^{Ψ_0} to a pure state $|\varphi_0\rangle\varphi_0|$. Furthermore we have to restrict the scaling behavior of the interaction to $\beta < 1/3$.

As it seems one needs these assumptions not only for technical reasons. Without them there might be regimes where clustering of the particle leads to a break down of the Gross-Pitaevskii description. It is clear that such a clustering can be avoided by assuming a high purity of the condensate (i.e. fast convergence of μ^{Ψ_0} to $|\varphi_0\rangle\varphi_0|$) and moderate scaling behavior of the interaction.

2 Counting the bad particles

We wish to control the number of bad particles in the condensate (i.e. the particles not in the state φ^t) using the method presented in [6]. Following [6] we need to define some projectors first which we will do next. We shall also give some general properties of these projectors before turning to the special case of deriving the Gross-Pitaevskii equation.

Definition 2.1. *Let* $\varphi \in L^2(\mathbb{R}^3 \to \mathbb{C})$.

(a) For any $1 \le j \le N$ *the projectors* $p_j^\varphi : L^2(\mathbb{R}^{3N} \to \mathbb{C}) \to L^2(\mathbb{R}^{3N} \to \mathbb{C})$ *and* $q_j^\varphi : L^2(\mathbb{R}^{3N} \to \mathbb{C}) \to L^2(\mathbb{R}^{3N} \to \mathbb{C})$ *are given by*

$$p_j^\varphi \Psi_N = \varphi(x_j) \int \varphi^*(x_j)\Psi_N(x_1, \ldots, x_N) d^3x_j \quad \forall\, \Psi_N \in L^2(\mathbb{R}^{3N} \to \mathbb{C})$$

and $q_j^\varphi = 1 - p_j^\varphi$.
We shall also use the bra-ket notation $p_j^\varphi = |\varphi(x_j)\rangle\langle\varphi(x_j)|$.

(b) For any $0 \le k \le j \le N$ *we define the set*

$$\mathcal{A}_k^j := \{(a_1, a_2, \ldots, a_j) : a_l \in \{0,1\}\ ;\ \sum_{l=1}^j a_l = k\}$$

and the orthogonal projector $P^{\varphi}_{j,k}$ *acting on* $L^2(\mathbb{R}^{3N} \to \mathbb{C})$ *as*

$$P^{\varphi}_{j,k} := \sum_{a \in \mathcal{A}^j_k} \prod_{l=1}^{j} \left(p^{\varphi}_{N-j+l}\right)^{1-a_l} \left(q^{\varphi}_{N-j+l}\right)^{a_l}$$

and denote the special case $j = N$ *by* $P^{\varphi}_k := P^{\varphi}_{N,k}$*. For negative* k *and* $k > j$ *we set* $P^{\varphi}_{j,k} := 0$*.*

(c) *For any function* $f : \{0, 1, \ldots, N\} \to \mathbb{R}^+_0$ *we define the operator* $\widehat{f}^{\varphi} : L^2(\mathbb{R}^{3N} \to \mathbb{C}) \to L^2(\mathbb{R}^{3N} \to \mathbb{C})$ *as*

$$\widehat{f}^{\varphi} := \sum_{j=0}^{N} f(j) P^{\varphi}_j \ . \tag{4}$$

We shall also need the shifted operators $\widehat{f}^{\varphi}_d : L^2(\mathbb{R}^{3N} \to \mathbb{C}) \to L^2(\mathbb{R}^{3N} \to \mathbb{C})$ *given by*

$$\widehat{f}^{\varphi}_d := \sum_{j=d}^{N+d} f(j+d) P^{\varphi}_j \ .$$

Notation. *Throughout the paper hats* $\widehat{\cdot}$ *shall solemnly be used in the sense of Definition 2.1 (c). The label* n *shall always be used for the function* $n(k) = \sqrt{k/N}$*.*

With Definition 2.1 we arrive directly at the following Lemma based on combinatorics of the p^{φ}_j and q^{φ}_j:

Lemma 2.2. (a) *For any functions* $f, g\{0, 1, \ldots, N\} \to \mathbb{R}^+_0$ *we have that*

$$\widehat{f}\widehat{g} = \widehat{fg} = \widehat{g}\widehat{f} \qquad \widehat{f} p_j = p_j \widehat{f} \qquad \widehat{f} P_{j,k} = P_{j,k} \widehat{f} \ .$$

(b) *Let* $n : \{0, 1, \ldots, N\} \to \mathbb{R}^+_0$ *be given by* $n(k) := \sqrt{k/N}$*. Then the square of* $\widehat{n}^{\varphi}$ *(c.f. (4)) equals the relative particle number operator of particles not in the state* φ*, i.e.*

$$(\widehat{n}^{\varphi})^2 = N^{-1} \sum_{j=1}^{N} q^{\varphi}_j \ .$$

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

$$\left\| \widehat{f}^{\varphi} q^{\varphi}_1 \Psi \right\|^2 = \| \widehat{f}^{\varphi} \widehat{n}^{\varphi} \Psi \|^2 \tag{5}$$

$$\left\| \widehat{f}^{\varphi} q^{\varphi}_1 q^{\varphi}_2 \Psi \right\|^2 \leq \frac{N}{N-1} \| \widehat{f}^{\varphi} (\widehat{n}^{\varphi})^2 \Psi \|^2 \ . \tag{6}$$

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

$$\widehat{f}^{\varphi} Q_j^{\varphi} v(x_1, x_2) Q_k^{\varphi} = Q_j^{\varphi} v(x_1, x_2) \widehat{f}_{j-k}^{\varphi} Q_k^{\varphi} \ ,$$

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 2.1, using that p_j and q_j are orthogonal projectors.

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

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

and (b) follows.

Let $\langle\!\langle \cdot, \cdot \rangle\!\rangle$ be the scalar product on $L^2(\mathbb{R}^{3N} \to \mathbb{C})$. For (5) we can write using symmetry of Ψ

$$\begin{aligned} \|\widehat{f}^{\varphi} \widehat{n}^{\varphi} \Psi\|^2 &= \langle\!\langle \Psi, (\widehat{f}^{\varphi})^2 (\widehat{n}^{\varphi})^2 \Psi \rangle\!\rangle = N^{-j} \sum_{k=1}^{N} \langle\!\langle \Psi, (\widehat{f}^{\varphi})^2 q_k^{\varphi} \Psi \rangle\!\rangle \\ &= \langle\!\langle \Psi, (\widehat{f}^{\varphi})^2 q_1^{\varphi} \Psi \rangle\!\rangle = \langle\!\langle \Psi, q_1^{\varphi} (\widehat{f}^{\varphi})^2 q_1^{\varphi} \Psi \rangle\!\rangle = \|(\widehat{f}^{\varphi}) q_1^{\varphi} \Psi\|^2 \ . \end{aligned}$$

Similarly we have for (6)

$$\begin{aligned} \|\widehat{f}^{\varphi} (\widehat{n}^{\varphi})^2 \Psi\|^2 &= \langle\!\langle \Psi, (\widehat{f}^{\varphi})^2 (\widehat{n}^{\varphi})^4 \Psi \rangle\!\rangle = N^{-2} \sum_{j,k=1}^{N} \langle\!\langle \Psi, (\widehat{f}^{\varphi})^2 q_j^{\varphi} q_k^{\varphi} \Psi \rangle\!\rangle \\ &= \frac{N-1}{N} \langle\!\langle \Psi, (\widehat{f}^{\varphi})^2 q_1^{\varphi} q_2^{\varphi} \Psi \rangle\!\rangle + N^{-1} \langle\!\langle \Psi, (\widehat{f}^{\varphi})^2 q_1^{\varphi} \Psi \rangle\!\rangle \\ &= \frac{N-1}{N} \|\widehat{f}^{\varphi} q_1^{\varphi} q_2^{\varphi} \Psi\| + N^{-1} \|\widehat{f}^{\varphi} q_1^{\varphi} \Psi\| \end{aligned}$$

and (c) follows.

Using the definitions above we have for (d)

$$\begin{aligned} \widehat{f}^{\varphi} Q_j^{\varphi} v(x_1, x_2) Q_k^{\varphi} &= \sum_{l=0}^{N} f(l) P_l^{\varphi} Q_j^{\varphi} v(x_1, x_2) Q_k^{\varphi} \\ &= \sum_{l=0}^{N} f(l) P_{N-2, l-j}^{\varphi} Q_j^{\varphi} v(x_1, x_2) Q_k^{\varphi} \\ &= \sum_{l=k-j}^{N+k-j} Q_j^{\varphi} v(x_1, x_2) f(l + j - k) P_{N-2, l-k}^{\varphi} Q_k^{\varphi} \end{aligned}$$

$$= \sum_{l=k-j}^{N+k-j} Q_j^{\varphi} v(x_1, x_2) f(l + j - k) P_l^{\varphi} Q_k^{\varphi} = Q_j^{\varphi} v(x_1, x_2) \widehat{f}_{j-k}^{\varphi} Q_k^{\varphi} \ .$$

□

3 Derivation of the Gross-Pitaevskii equation

As presented in [6] we wish to control the functional $\alpha_N : (L^2(\mathbb{R}^{3N} \to \mathbb{C}) \times L^2(\mathbb{R}^3 \to \mathbb{C}) \to \mathbb{R}_0^+)$ given by

$$\alpha_N(\Psi, \varphi) = \langle \Psi, \widehat{m}^\varphi \Psi \rangle$$

for some appropriate weight $m : \{0, \ldots, N\} \to \mathbb{R}_0^+$.

As mentioned above we shall need comparably strong conditions on the "purity" of the initial condensate to derive the Gross-Pitaevskii equation without positivity assumption on the interaction. This is encoded in the weights we shall choose below (see Definition 3.1). For these weights convergence of the respective α is stronger than $\mu^\Psi \to |\varphi\rangle\langle\varphi|$ in operator norm (see Lemma 3.3).

Note that we shall allow rather general interactions (even negative interactions) and that the Theorem below is useless when the solution of the Gross-Pitaevskii equation does not behave nicely. There is a lot of literature on solutions of nonlinear Schrödinger equation (see for example [3]) showing that at least for positive $a = \int v(x) d^3x$ our assumptions on the solutions of the Gross-Pitaevskii equation can be satisfied for many different setups.

Definition 3.1. *For any $0 < \lambda < 1$ we define the function $m^\lambda : \{1, \ldots, N\} \to \mathbb{R}_0^+$ given by*

$$m^\lambda(k) := \begin{cases} k/N^\lambda, & \text{for } k \leq N^\lambda; \\ 1, & \text{else.} \end{cases}$$

We define for any $N \in \mathbb{N}$ the functional $\alpha_N^\lambda : L^2(\mathbb{R}^{3N} \to \mathbb{C}) \times L^2(\mathbb{R}^3 \to \mathbb{C}) \to \mathbb{R}_0^+$ by

$$\alpha_N^\lambda(\Psi_N, \varphi) := \langle\!\langle \Psi_N, \widehat{m}^{\lambda,\varphi} \Psi_N \rangle\!\rangle = \|(\widehat{m}^{\lambda,\varphi})^{1/2} \Psi_N\|^2 .$$

With these definitions we arrive at the main Theorem:

Theorem 3.2. *Let $0 < \lambda, \beta < 1$, let $v_N^\beta(x)$ satisfy assumption 1.1. Let $0 < T \leq \infty$, let A^t be a time dependent potential. Assume that for any $N \in \mathbb{N}$ there exists a solution of the Schrödinger equation Ψ_N^t and a L^∞ solution of the Gross-Pitaevskii equation (3) φ^t with $\Delta|\varphi^t|^2 \in L^2$ for all $0 \leq t \leq T$. Then*

$$\alpha_N^\lambda(\Psi_N^t, \varphi^t) \leq e^{\int_0^t C_v \|\varphi^s\|_\infty^2 ds} \alpha_N^\lambda(\Psi_N^0, \varphi^0) + (e^{\int_0^t C_v \|\varphi^s\|_\infty^2 ds} - 1) K^{\varphi^t} N^{-\delta_\lambda} ,$$

where $\delta_\lambda = \frac{1}{2} \max\{1 - \lambda - 4\beta \, , \ -1 + \lambda + 3\beta\}$, C_v is some constant depending on v only and

$$K^\varphi := C_v \left(\|\Delta|\varphi|^2\| + \|\varphi\|_\infty + 1 \right) \|\varphi\|_\infty .$$

The proof of the Theorem shall be given below.

Remark. *For $\beta < 1/3$ one can choose λ such that δ_λ is negative.*

3.1 Convergence of the reduced density matrix

In [6] Lemma 2.2 it is shown that convergence of $\alpha_N(\Psi,\varphi)\to 0$ is equivalent to convergence of the reduced one particle marginal density to $|\varphi\rangle\langle\varphi|$ in trace norm for many different weights. The weights we use here are not covered by that Lemma. Since $m^\lambda(k)\geq k/N$ for all $0\leq k\leq N$ and all $0<\lambda<1$ it follows that $\alpha_N^\lambda(\Psi,\varphi)\geq\langle\!\langle\Psi,\widehat{n}^2\Psi\rangle\!\rangle$ (recall that $n(k)=\sqrt{k/N}$). It follows with Lemma 2.2 in [6] that for all $0<\lambda<1$

$$\lim_{N\to\infty}\alpha_N^\lambda(\Psi,\varphi)=0\quad\Rightarrow\lim_{N\to\infty}\mu^\Psi\to|\varphi\rangle\langle\varphi|\ \text{ in operator norm.}$$

Therefore our result implies convergence of the respective reduced one particle marginal density. To be able to formulate Theorem 3.2 under conditions of the reduced one particle marginal density we have the following Lemma

Lemma 3.3. *Let $0<\lambda<1$, $\xi<0$ and let $\|\mu^\Psi-|\varphi\rangle\langle\varphi|\|_{op}=\mathcal{O}(N^\xi)$. Then*

$$\alpha_N^\lambda(\Psi,\varphi)=\mathcal{O}(N^{1-\lambda+\xi})\ .$$

Proof. Under the assumptions of the Lemma it follows that $\langle\varphi,\mu^\Psi\varphi\rangle=\mathcal{O}(N^\xi)$. Writing

$$\begin{aligned}\mu^{\Psi_N} &= \int\Psi_N(\cdot,x_2,\ldots,x_N)\Psi_N^*(\cdot,x_2,\ldots,x_N)d^{3N-3}x\\ &= \int p_1^\varphi\Psi_N(\cdot,x_2,\ldots,x_N)p_1^\varphi\Psi_N^*(\cdot,x_2,\ldots,x_N)d^{3N-3}x\\ &\quad+\int q_1^\varphi\Psi_N(\cdot,x_2,\ldots,x_N)p_1^\varphi\Psi_N^*(\cdot,x_2,\ldots,x_N)d^{3N-3}x\\ &\quad+\int p_1^\varphi\Psi_N(\cdot,x_2,\ldots,x_N)q_1^\varphi\Psi_N^*(\cdot,x_2,\ldots,x_N)d^{3N-3}x\\ &\quad+\int q_1^\varphi\Psi_N(\cdot,x_2,\ldots,x_N)q_1^\varphi\Psi_N^*(\cdot,x_2,\ldots,x_N)d^{3N-3}x\end{aligned}$$

and using $q_1^\varphi\varphi(x_1)=0$ it follows that $\|p_1^\varphi\Psi_N\|^2-1=\mathcal{O}(N^\xi)$. Using $p_1^\varphi+q_1^\varphi=1$ and Lemma 2.2 (c)

$$\|q_1^\varphi\Psi_N\|^2=\langle\!\langle\Psi,\widehat{n}^2\Psi\rangle\!\rangle=\left\langle\!\!\left\langle\Psi,\sum_{k=0}^N\frac{k}{N}P_k^\varphi\Psi\right\rangle\!\!\right\rangle=\mathcal{O}(N^\xi)\ .$$

Since $m^\lambda(k)\leq N^{1-\lambda}k/N$ for any $0\leq k\leq N$ it follows that

$$\alpha_N^\lambda(\Psi,\varphi)\leq N^{1-\lambda}\left\langle\!\!\left\langle\Psi,\sum_{k=0}^N\frac{k}{N}P_k^\varphi\Psi\right\rangle\!\!\right\rangle=\mathcal{O}(N^{1-\lambda+\xi})\ .$$

□

3.2 Proof of the Theorem

In our estimates below we shall need from time to time the operator norm $\|\cdot\|_{op}$ defined for any linear operator $f : L^2(\mathbb{R}^{3N} \to \mathbb{C}) \to L^2(\mathbb{R}^{3N} \to \mathbb{C})$ by

$$\|f\|_{op} := \sup_{\|\Psi\|=1} \|f\Psi\| \; .$$

In particular we shall need the following Proposition

Proposition 3.4. *(a) For any $f \in L^2(\mathbb{R}^3 \to \mathbb{C})$*

$$\|f(x_1 - x_2)p_1^\varphi\|_{op} \leq \|\varphi\|_\infty \|f\| \; .$$

(b) For any $g \in L^1(\mathbb{R}^3 \to \mathbb{C})$

$$\|p_1^\varphi g(x_1 - x_2)p_1^\varphi\|_{op} \leq \|\varphi\|_\infty^2 \|g\|_1 \; .$$

Proof. (a): Let $f \in L^2(\mathbb{R}^3 \to \mathbb{C})$. Using the notation $p_1^\varphi = |\varphi(x_1)\rangle\langle\varphi(x_1)|$

$$\begin{aligned}
\|f(x_1 - x_2)p_1^\varphi\|_{op}^2 &= \sup_{\|\Psi\|=1} \|f(x_1 - x_2)p_1^\varphi\Psi\|^2 \\
&= \sup_{\|\Psi\|=1} \langle\!\langle \Psi, |\varphi(x_1)\rangle\langle\varphi(x_1)|f(x_1 - x_2)^2|\varphi(x_1)\rangle\langle\varphi(x_1)|\Psi\rangle\!\rangle \; .
\end{aligned}$$

Using that

$$\sup_{x_2 \in \mathbb{R}^3} \langle\varphi(x_1)|f(x_1 - x_2)^2|\varphi(x_1)\rangle \leq \|\varphi\|_\infty^2 \|f\|^2$$

and Cauchy Schwarz one gets

$$\|f(x_1 - x_2)p_1^\varphi\|_{op}^2 \leq \sup_{\|\Psi\|=1} \|\Psi\|^2 \|\varphi\|_\infty^2 \|f\|^2 \; .$$

(b): Let $g \in L^1(\mathbb{R}^3 \to \mathbb{C})$.

$$\begin{aligned}
\|p_1^\varphi g(x_1 - x_2)p_1^\varphi\|_{op} &\leq \|p_1^\varphi |g(x_1 - x_2)| p_1^\varphi\|_{op} \\
&= \|p_1^\varphi \sqrt{|g(x_1 - x_2)|}\sqrt{|g(x_1 - x_2)|}p_1^\varphi\|_{op} \\
&\leq \|\sqrt{|g(x_1 - x_2)|}p_1^\varphi\|_{op}^2 \; .
\end{aligned}$$

With (a) we get (b).

□

We prove the Theorem using a Grønwall argument. Therefore we estimate $\dot{\alpha}_N^\lambda(\Psi_N^t, \varphi^t)$ in terms of $\alpha_N^\lambda(\Psi_N^t, \varphi^t)$. To get the estimates as stated in Theorem 3.2 we need to show that

$$|\dot{\alpha}_N^\lambda(\Psi_N^t, \varphi^t)| \leq C_v \|\varphi^t\|_\infty^2 \alpha_N^\lambda(\Psi_N^t, \varphi^t) + K^{\varphi^t} N^{-\delta} \; . \tag{7}$$

To shorten notation we use the following definitions:

Definition 3.5. *Let*

$$h_{j,k} := N(N-1)v_N^\beta(x_j-x_k) - aN|\varphi|^2(x_j) - aN|\varphi|^2(x_k)\ .$$

We define the functional $\gamma_N^\lambda : L^2(\mathbb{R}^{3N} \to \mathbb{C}) \to \mathbb{R}$ *by*

$$\begin{aligned}\gamma_N^\lambda(\Psi,\varphi) \quad &= \quad 2\Im\left(\langle\!\langle \Psi, (\widehat{m}_{-1}^{\lambda,\varphi} - \widehat{m}^{\lambda,\varphi})p_1q_2h_{1,2}p_1p_2\Psi\rangle\!\rangle\right)\\ &\quad +\Im\left(\langle\!\langle \Psi, q_1q_2h_{1,2}(\widehat{m}^{\lambda,\varphi} - \widehat{m}_2^{\lambda,\varphi})p_1p_2\Psi\rangle\!\rangle\right)\\ &\quad +2\Im\left(\langle\!\langle \Psi, (\widehat{m}_{-1}^{\lambda,\varphi} - \widehat{m}^{\lambda,\varphi})q_1q_2h_{1,2}p_1q_2\Psi\rangle\!\rangle\right)\ .\end{aligned}$$

γ_N^λ was defined in such a way that for any solution of the Schrödinger equation Ψ_N^t and any solution φ^t of the Gross-Pitaevskii equation $\dot{\alpha}_N^\lambda(\Psi_N^t,\varphi^t) = \gamma_N^\lambda(\Psi_N^t,\varphi^t)$ (see Lemma 3.6 below). It is left to show that $\gamma_N^\lambda(\Psi_N^t,\varphi^t)$ can be controlled by $\alpha_N^\lambda(\Psi_N^t,\varphi^t)$ and $N^{-\delta}$ (which is done in Lemma 3.7 below) to get (7) and – via Grønwall – the Theorem.

Lemma 3.6. *For any solution of the Schrödinger equation* Ψ_N^t*, any solution of the Gross-Pitaevskii equation* φ^t *and any* $0<\lambda<1$ *we have*

$$\dot{\alpha}_N^\lambda(\Psi_N^t,\varphi^t) = \gamma_N^\lambda(\Psi_N^t,\varphi^t)\ .$$

Proof. Let

$$H_{GP}^\varphi := \sum_{k=1}^N -\Delta_k + A(x_k) + a|\varphi|^2(x_k)$$

be the sum of Gross-Pitaevskii Hamiltonians in each particle. It follows that

$$\frac{d}{dt}\widehat{f}^{\varphi^t} = i[H_{GP}^{\varphi^t}, \widehat{f}^{\varphi^t}] \tag{8}$$

for any function $f : \{0,\ldots,N\} \to \mathbb{R}$. For ease of notation we shall drop now the indices φ and λ for the rest of the proof. With (8) we get

$$\begin{aligned}\dot{\alpha}_N(\Psi_N^t,\varphi^t) \quad &= \quad i\langle\!\langle \Psi_N^t, \widehat{m}H\Psi_N^t\rangle\!\rangle - i\langle\!\langle H\Psi_N^t, \widehat{m}\Psi_N^t\rangle\!\rangle + i\langle\!\langle \Psi_N^t, [H_{GP},\widehat{m}]\Psi_N^t\rangle\!\rangle\\ &= \quad -i\langle\!\langle \Psi_N^t, [H-H_{GP},\widehat{m}]\Psi_N^t\rangle\!\rangle\ .\end{aligned}$$

Using symmetry of Ψ_N^t and selfadjointness of $h_{j,k}$ it follows that

$$\begin{aligned}\dot{\alpha}_N(\Psi_N^t,\varphi^t) \quad &= \quad -i(N^2-N)^{-1}\sum_{1\le j<k\le N}\langle\!\langle \Psi_N^t, [h_{j,k},\widehat{m}\ ]\Psi_N^t\rangle\!\rangle\\ &= \quad -\frac{i}{2}\left(\langle\!\langle \Psi_N^t, h_{1,2}\widehat{m}\ \Psi_N^t\rangle\!\rangle - \langle\!\langle \Psi_N^t, \widehat{m}\ h_{1,2}\Psi_N^t\rangle\!\rangle\right)\\ &= \quad \Im\left(\langle\!\langle \Psi_N^t, h_{1,2}\widehat{m}\ \Psi_N^t\rangle\!\rangle\right)\ .\end{aligned} \tag{9}$$

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

$$\begin{aligned}
\widehat{m} &= \sum_{k=0}^{N} m(k)P_k \\
&= \sum_{k=0}^{N-2}\big(m(k)p_1p_2P_{N-2,k}+m(k)p_1q_2P_{N-2,k-1} \\
&\quad +m(k)q_1p_2P_{N-2,k-1}+m(k)(1-p_1q_2-q_1p_2-p_1p_2)P_{N-2,k-2}\big) \\
&= \sum_{k=0}^{N}\big(m(k)p_1p_2P_{N-2,k}+m(k)p_1q_2P_{N-2,k-1} \\
&\quad +m(k)q_1p_2P_{N-2,k-1}+m(k)P_{N-2,k-2}\big) \\
&\quad -\sum_{k=0}^{N} m(k+1)p_1q_2P_{N-2,k-1}-m(k+1)q_1p_2P_{N-2,k-1} \\
&\quad -m(k+2)p_1p_2P_{N-2,k}\big) \\
&= (\widehat{m}-\widehat{m}_2)p_1p_2+(\widehat{m}-\widehat{m}_1)p_1q_2+(\widehat{m}-\widehat{m}_1)q_1p_2 \\
&\quad +\sum_{k=0}^{N} m(k)P_{N-2,k-2}\ . \qquad (10)
\end{aligned}$$

Using symmetry of Ψ_N^t and selfadjointness of $h_{1,2}P_{N-2,k-2}$ it follows that

$$\dot{\alpha}_N(\Psi_N^t,\varphi^t)=\Im\left(\langle\!\langle\Psi_N^t,h_{1,2}\left((\widehat{m}-\widehat{m}_2)p_1p_2+2(\widehat{m}-\widehat{m}_1)p_1q_2\right)\Psi_N^t\rangle\!\rangle\right)\ . \qquad (11)$$

Since $1=p_1p_2+p_1q_2+q_1p_2+q_1q_2$

$$\begin{aligned}
\dot{\alpha}_N(\Psi_N^t,\varphi^t) &= \Im\left(\langle\!\langle\Psi,p_1p_2h_{1,2}(\widehat{m}-\widehat{m}_2)p_1p_2\Psi\rangle\!\rangle\right) \\
&\quad +\Im\left(\langle\!\langle\Psi,p_1q_2h_{1,2}(\widehat{m}-\widehat{m}_2)p_1p_2\Psi\rangle\!\rangle\right) \\
&\quad +\Im\left(\langle\!\langle\Psi,q_1p_2h_{1,2}(\widehat{m}-\widehat{m}_2)p_1p_2\Psi\rangle\!\rangle\right) \\
&\quad +\Im\left(\langle\!\langle\Psi,q_1q_2h_{1,2}(\widehat{m}-\widehat{m}_2)p_1p_2\Psi\rangle\!\rangle\right) \\
&\quad +2\Im\left(\langle\!\langle\Psi,p_1p_2h_{1,2}(\widehat{m}-\widehat{m}_1)p_1q_2\Psi\rangle\!\rangle\right) \\
&\quad +2\Im\left(\langle\!\langle\Psi,p_1q_2h_{1,2}(\widehat{m}-\widehat{m}_1)p_1q_2\Psi\rangle\!\rangle\right) \\
&\quad +2\Im\left(\langle\!\langle\Psi,q_1p_2h_{1,2}(\widehat{m}-\widehat{m}_1)p_1q_2\Psi\rangle\!\rangle\right) \\
&\quad +2\Im\left(\langle\!\langle\Psi,q_1q_2h_{1,2}(\widehat{m}-\widehat{m}_1)p_1q_2\Psi\rangle\!\rangle\right)\ .
\end{aligned}$$

Using that $\Im(\langle\!\langle\Psi,A\Psi\rangle\!\rangle)=-\Im(\langle\!\langle\Psi,A^t\Psi\rangle\!\rangle)$ for any operator A and that Ψ is symmetric (note that $p_1q_2h_{1,2}q_1p_2$ is invariant under adjunction with simultaneous exchange of the variables x_1 and x_2) and Lemma 2.2 (d) we get

$$\begin{aligned}
\dot{\alpha}_N(\Psi_N^t,\varphi^t) &= 2\Im\left(\langle\!\langle\Psi,p_1q_2h_{1,2}(\widehat{m}-\widehat{m}_2)p_1p_2\Psi\rangle\!\rangle\right) \\
&\quad -2\Im\left(\langle\!\langle\Psi,p_1q_2(\widehat{m}-\widehat{m}_1)h_{1,2}p_1p_2\Psi\rangle\!\rangle\right) \\
&\quad +\Im\left(\langle\!\langle\Psi,q_1q_2h_{1,2}(\widehat{m}-\widehat{m}_2)p_1p_2\Psi\rangle\!\rangle\right) \\
&\quad +2\Im\left(\langle\!\langle\Psi,q_1q_2h_{1,2}(\widehat{m}-\widehat{m}_1)p_1q_2\Psi\rangle\!\rangle\right)\ .
\end{aligned}$$

Lemma 2.2 (d) applied to the first and fourth summand completes the proof. □

With Lemma 3.6 equation (7) follows once we can control the different summands appearing in γ_N^λ in a suitable way. So the following Lemma completes the proof of the Theorem.

Lemma 3.7. *Let v_N^β satisfy assumption 1.1. Then there exists a $C<\infty$ such that for any $\varphi \in L^\infty$ with $\Delta|\varphi|^2 \in L^2$*

(a)

$$\left|\langle\!\langle \Psi, (\widehat{m}_{-1}^{\lambda,\varphi} - \widehat{m}^{\lambda,\varphi}) p_1 q_2 h_{1,2} p_1 p_2 \Psi \rangle\!\rangle\right| \leq K^\varphi N^{\delta_\lambda}$$

(b)

$$\left|\langle\!\langle \Psi, q_1 q_2 h_{1,2} (\widehat{m}^{\lambda,\varphi} - \widehat{m}_{2}^{\lambda,\varphi}) p_1 p_2 \Psi \rangle\!\rangle\right| \leq C\|\varphi\|_\infty^2 \alpha_N^\lambda(\Psi,\varphi) + K^\varphi N^{\delta_\lambda}$$

(c)

$$\left|\langle\!\langle \Psi, (\widehat{m}_{-1}^{\lambda,\varphi} - \widehat{m}^{\lambda,\varphi}) q_1 q_2 h_{1,2} p_1 q_2 \Psi \rangle\!\rangle\right| \leq K^\varphi N^{\delta_\lambda}$$

with δ_λ and K^φ as in Theorem 3.2.

Before we prove the Lemma a few words on (a) and (c) first: It is (a) which is physically the most important. Here the mean field cancels out most of the interaction. The central point in the mean field argument is observing that $p_1 q_2 h_{1,2} p_1 p_2$ is small.

For (c) the choice of the weights m^λ plays an important role. Note that we only have one projector p here and $\|q_1 q_2 h_{1,2} p_1 q_2\|_{op}$ can not be controlled by the L^1-norm of v (see Proposition 3.4). On the other hand we have altogether three projectors q in (c). Assuming that the condensate is very clean (which is encoded in $\widehat{m}^\lambda$) these q's make (c) small.

Proof. In the proof we shall drop the index λ and φ for ease of notation. Constants appearing in estimates will generically be denoted by C. We shall not distinguish constants appearing in a sequence of estimates, i.e. in $X \leq CY \leq CZ$ the constants may differ.

In bra-ket notation $p_1 = |\varphi(x_1)\rangle\langle\varphi(x_1)|$. Writing $\star$ for the convolution we get for any $f:\mathbb{R}^6 \to \mathbb{R}$

$$p_1 f(x_1-x_2) p_1 = |\varphi(x_1)\rangle\langle\varphi(x_1)| f(x_1-x_2) |\varphi(x_1)\rangle\langle\varphi(x_1)| = p_1 (f \star |\varphi|^2)(x_2) \;, \tag{12}$$

in particular

$$p_1 \delta(x_1-x_2) p_1 = p_1 |\varphi(x_2)|^2 \;.$$

With $p_1 q_1 = 0$ it follows that

$$\begin{aligned} p_1 q_2 h_{1,2} p_1 p_2 &= N p_1 q_2 \Big((N-1) v_N^\beta (x_1-x_2) - a|\varphi|^2(x_2) \Big) p_1 p_2 \\ &= N p_1 q_2 \Big((N-1) v_N^\beta (x_1-x_2) - a\delta(x_1-x_2) \Big) p_1 p_2 \;. \end{aligned}$$

Using this and triangle inequality the left hand side of (a) is bounded by

$$N|\langle\langle \Psi, (\widehat{m}_{-1} - \widehat{m}) p_1 q_2 \left(N v_N^\beta (x_1 - x_2) - a\delta(x_1 - x_2) \right) p_1 p_2 \Psi \rangle\rangle| + N|\langle\langle \Psi, (\widehat{m}_{-1} - \widehat{m}) p_1 q_2 v_N^\beta (x_1 - x_2) p_1 p_2 \Psi \rangle\rangle| \; . \tag{13}$$

To control the first summand we define the function $f_N^\beta : \mathbb{R}^3 \to \mathbb{R}$ by

$$\Delta f_N^\beta = N v_N^\beta - a\delta \; .$$

Recall that v is compactly supported. Since $N \int v(x) d^3x = a$ the integration constant of f_N^β can be chosen such that also f_N^β has compact support. Using the scaling behavior of v_N^β it follows that there exits a function $f : \mathbb{R}^3 \to \mathbb{R}$ with

$$f_N^\beta = N^\beta f(N^\beta x) \qquad \text{and} \qquad \|f_N^\beta\|_1 = N^{-2\beta} \|f\|_1 \; .$$

Now we can estimate the first summand in (13) using (12)

$$\begin{aligned}
& N|\langle\langle \Psi, (\widehat{m}_{-1} - \widehat{m}) p_1 q_2 \Delta f_N^\beta (x_1 - x_2) p_1 p_2 \Psi \rangle\rangle| \\
= \;& N|\langle\langle \Psi, (\widehat{m}_{-1} - \widehat{m}) p_1 q_2 \left((\Delta f_N^\beta) \star |\varphi|^2 \right) (x_2) p_1 p_2 \Psi \rangle\rangle| \\
= \;& N|\langle\langle \Psi, (\widehat{m}_{-1} - \widehat{m}) p_1 q_2 \left(f_N^\beta \star (\Delta |\varphi|^2) \right) (x_2) p_1 p_2 \Psi \rangle\rangle| \; .
\end{aligned}$$

Since $\|p_1 p_2 \Psi\| \leq 1$ one gets with Proposition 3.4

$$\begin{aligned}
\leq \;& N \|(\widehat{m}_{-1} - \widehat{m}) q_2 \Psi\| \; \|p_1 \left(f_N^\beta \star (\Delta |\varphi|^2) \right) (x_2) p_1\|_{op} \\
\leq \;& N \|(\widehat{m}_{-1} - \widehat{m}) q_2 \Psi\| \; \|f_N^\beta \star (\Delta |\varphi|^2)\| \; \|\varphi\|_\infty \; .
\end{aligned}$$

In view of Lemma 2.1 (b) we have using symmetry of Ψ for the first factor

$$\begin{aligned}
\|(\widehat{m}_{-1} - \widehat{m}) q_2 \Psi\| &= \|(\widehat{m}_{-1} - \widehat{m}) \widehat{n} \Psi\| \\
&\leq \sup_{0 \leq k \leq N^\lambda} \left(\left| \frac{k-1}{N^\lambda} - \frac{k}{N^\lambda} \right| \sqrt{k/N} \right) = (N^\lambda N)^{-1/2} \; .
\end{aligned} \tag{14}$$

Using Young's inequality we have for the second factor

$$\|f_N^\beta \star (\Delta |\varphi|^2)\| \leq \|f_N^\beta\|_1 \; \|\Delta |\varphi|^2\| \; \leq \; C N^{-2\beta} \; \|\Delta |\varphi|^2\| \; .$$

It follows that the first summand of (13) is bounded by

$$C N^{-\lambda/2} \|\Delta |\varphi|^2\| \; \|\varphi\|_\infty N^{1/2 - 2\beta} \; . \tag{15}$$

Using Schwarz inequality, then Proposition 3.4 and equation (14) the second summand of (13) is smaller than

$$\begin{aligned}
& N \|(\widehat{m}_{-1} - \widehat{m}) q_2 \Psi\| \; \|p_1 v_N^\beta (x_1 - x_2) p_1\|_{op} \\
\leq \;& N \|(\widehat{m}_{-1} - \widehat{m}) q_2 \Psi\| \; \|v_N^\beta\|_1 \; \|\varphi\|_\infty^2 \leq C (N^\lambda N)^{-1/2} \|\varphi\|_\infty^2 \; .
\end{aligned}$$

Using this and (15) we get (a).

For (b) we use first that $q_1q_2w(x_1)p_1p_2=0$ for any function w. It follows with Lemma 2.1 (d) that

$$\begin{aligned}
&\langle\!\langle \Psi, q_1q_2h_{1,2}(\widehat{m}-\widehat{m}_2)p_1p_2\Psi\rangle\!\rangle \qquad (16)\\
=\;& (N^2-N)\langle\!\langle \Psi, q_1q_2(\widehat{m}_{-2}-\widehat{m})^{1/2}v_N^\beta(x_1-x_2)(\widehat{m}-\widehat{m}_2)^{1/2}p_1p_2\Psi\rangle\!\rangle\ .
\end{aligned}$$

Before we estimate this term note that the operator norm of $q_1q_2v_N^\beta(x_1-x_2)$ restricted to the subspace of symmetric functions is much smaller than the operator norm on full $L^2(\mathbb{R}^{3N}\to\mathbb{C})$. This comes from the fact that $v_N(x_1-x_2)$ is only nonzero in a small area where $x_1\approx x_2$. A non-symmetric wave function may be fully localized in that area, whereas for a symmetric wave function only a small part lies in that area. To get sufficiently good control of (16) we symmetrize $(N-1)v_N^\beta(x_1-x_2)$ replacing it by $\sum_{k=2}^N v_N^\beta(x_1-x_k)$ and get

$$\begin{aligned}
(16) \;&=\; (N^2-N)\langle\!\langle \Psi, q_1q_2(\widehat{m}_{-2}-\widehat{m})^{1/2}v_N^\beta(x_1-x_2)(\widehat{m}-\widehat{m}_2)^{1/2}p_1p_2\Psi\rangle\!\rangle\\
&=\; N\langle\!\langle \Psi, (\widehat{m}_{-2}-\widehat{m})^{1/2}\sum_{j=2}^N q_1q_jv_N^\beta(x_1-x_j)p_1p_j(\widehat{m}-\widehat{m}_2)^{1/2}\Psi\rangle\!\rangle\\
&\leq\; N\|(\widehat{m}_{-2}-\widehat{m})^{1/2}q_1\Psi\|\;\|\sum_{j=2}^N q_jv_N^\beta(x_1-x_j)p_1p_j(\widehat{m}-\widehat{m}_2)^{1/2}\Psi\|\ .
\end{aligned}$$

For the first factor we have since $(m(k)-m(k-2))\,k/N\leq 2N^{-1}m(k)$ in view of Lemma 2.2 (c) that

$$\|(\widehat{m}_{-2}-\widehat{m})^{1/2}q_1\Psi\|^2 \;=\; \langle\!\langle \Psi(\widehat{m}_{-2}-\widehat{m})\widehat{n}^2\Psi\rangle\!\rangle \;\leq\; 2N^{-1}\alpha_N(\Psi,\varphi)\ .$$

The second factor is bounded by

$$\begin{aligned}
&\sum_{2\leq j<k\leq N}^N \langle\!\langle (\widehat{m}-\widehat{m}_2)^{1/2}\Psi, p_1p_jv_N^\beta(x_1-x_j)q_jq_kv_N^\beta(x_1-x_k)(\widehat{m}-\widehat{m}_2)^{1/2}p_1p_k\Psi\rangle\!\rangle\\
&\quad+\sum_{k=2}^N \|q_kv_N^\beta(x_1-x_k)p_1p_k(\widehat{m}-\widehat{m}_2)^{1/2}\Psi\|^2\ . \qquad (17)
\end{aligned}$$

Using symmetry and Proposition 3.4 the first summand in (17) is bounded by

$$\begin{aligned}
&N^2\langle\!\langle (\widehat{m}-\widehat{m}_2)^{1/2}\Psi, p_1p_2q_3v_N^\beta(x_1-x_2)v_N^\beta(x_1-x_3)p_1q_2p_3(\widehat{m}-\widehat{m}_2)^{1/2}\Psi\rangle\!\rangle\\
&\leq\; N^2\|\sqrt{|v_N^\beta(x_1-x_2)|}\sqrt{|v_N^\beta(x_1-x_3)|}p_1q_2p_3(\widehat{m}-\widehat{m}_2)^{1/2}\Psi\|^2\\
&\leq\; N^2\|\sqrt{|v_N^\beta(x_1-x_2)|}p_1\|_{op}^4\;\|(\widehat{m}-\widehat{m}_2)^{1/2}q_2\Psi\|^2\\
&\leq\; N^2\|\varphi\|_\infty^4\|v_N^\beta\|_1^2\|(\widehat{m}-\widehat{m}_2)^{1/2}q_2\Psi\|^2\\
&\leq\; C\|\varphi\|_\infty^4\alpha_N(\Psi,\varphi)\ .
\end{aligned}$$

Using Proposition 3.4 the second summand in (17) can be controlled by

$$
\begin{aligned}
& N\langle\!\langle (\widehat{m}-\widehat{m}_2)^{1/2}\Psi, p_1p_2(v_N^\beta(x_1-x_2))^2 p_1p_2(\widehat{m}-\widehat{m}_2)^{1/2}\Psi\rangle\!\rangle \\
\leq\; & N\|p_1(v_N^\beta(x_1-x_2))^2p_1\|_{op}\, \|(\widehat{m}-\widehat{m}_2)^{1/2}\|_{op}^2 \\
\leq\; & N\|\varphi\|_\infty^2\, \|v_N^\beta\|_2^2\, \|(\widehat{m}-\widehat{m}_2)^{1/2}\|_{op}^2 \leq C\|\varphi\|_\infty^2 N N^{-2+3\beta}N^{-\lambda}\,.
\end{aligned}
$$

It follows that (b) is bounded by

$$
C\|\varphi\|_\infty^2\alpha_N(\Psi,\varphi)+C\|\varphi\|_\infty N^{-1/2+3/2\beta}N^{-\lambda/2}\,.
$$

Next we shall prove (c). Using Lemma 2.1 (d) and Cauchy-Schwarz we get for the left hand side of (c)

$$
\begin{aligned}
& \left|\langle\!\langle \Psi, (\widehat{m}_{-1}-\widehat{m})\widehat{n}_1 q_1q_2h_{1,2}\widehat{n}^{-1}p_1q_2\Psi\rangle\!\rangle\right| \\
& \qquad \leq \|(\widehat{m}_{-1}-\widehat{m})\widehat{n}_1q_1q_2\Psi\|\, \|h_{1,2}\widehat{n}^{-1}p_1q_2\Psi\|\,.
\end{aligned}
$$

For the first factor we have using Lemma 2.1 (c)

$$
\begin{aligned}
\|(\widehat{m}_{-1}-\widehat{m})\widehat{n}_1q_1q_2\Psi\| &\leq \frac{N}{N-1}\|(\widehat{m}_{-1}-\widehat{m})\widehat{n}_1\widehat{n}^2\Psi\| \\
&\leq \sup_{0\leq k\leq N^\lambda}\left(\frac{N}{N-1}\left|\frac{k-1}{N^\lambda}-\frac{k}{N^\lambda}\right|\sqrt{(k+1)/N}\frac{k}{N}\right) \\
&= \frac{\sqrt{N^\lambda+1}}{(N-1)\sqrt{N}}\,.
\end{aligned}
$$

For the second factor we have using Proposition 3.4 and Lemma 2.2 (c)

$$
\begin{aligned}
\|h_{1,2}\widehat{n}^{-1}p_1q_2\Psi\| &\leq \|h_{1,2}p_1\|_{op}\, \|\widehat{n}^{-1}q_2\Psi\| \\
&\leq \|\varphi\|_\infty\, \|h_{1,2}\| \leq N\|\varphi\|_\infty\, \Big((N-1)\|v_N^\beta\|+\|2a|\varphi|^2\|\Big)\,.
\end{aligned}
$$

Since the scaling of v_N^β is such that $\|v_N^\beta\|=\|v\|N^{-1+3/2\beta}$ it follows that (c) is bounded by

$$
\begin{aligned}
& CN\frac{\sqrt{N^\lambda+1}}{(N-1)\sqrt{N}}(N-1)N^{-1+3/2\beta}(\|\varphi\|_\infty+\|\varphi\|_\infty^2) \\
& \leq C(\|\varphi\|_\infty+\|\varphi\|_\infty^2)N^{\lambda/2}N^{-1/2+3/2\beta}
\end{aligned}
$$

and (c) follows.

□

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