Derivation of the Time Dependent Gross-Pitaevskii Equation Without Positivity Condition on the Interaction

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Abstract Using a new method (Pickl in A simple derivation of mean field limits for quantum systems, 2010) 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 (Erdös et al. in Commun. Pure Appl. Math. 59(12):1659–1741, 2006; Invent. Math. 167:515–614, 2007). The new method for dealing with mean field limits presented in Pickl (2010) 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 of the interaction and that we have to assume fast convergence of the reduced one particle marginal density matrix of the initial wave function \( \mu \Psi_0 \) to a pure state \( |\psi_0\rangle \langle \psi_0| \).

Keywords Mean field limits · Gross-Pitaevskii equation · BEC

1 Introduction

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

\[
i \Psi_N' = H_N \Psi_N'
\]

(1)

with symmetric \( \Psi_N^0 \) we shall specify below and the Hamiltonian

\[
H_N = -\sum_{j=1}^{N} \Delta_j + \sum_{1 \leq j < k \leq N} v_N^\beta(x_j - x_k) + \sum_{j=1}^{N} A^j(x_j)
\]

(2)

acting on the Hilbert space \( L^2(\mathbb{R}^{3N}) \). \( \beta \in \mathbb{R} \) stands for the scaling behavior of the interaction. The \( v_N^\beta \) 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

\[ v^\beta_N(x) = N^{-1+3\beta} v(N^\beta x) \]
with compactly supported, spherically symmetric \( v \in L^\infty \).

The trap potential \( A \) does not depend on \( N \). \( H_N \) conserves symmetry, i.e. any symmetric function \( \Psi^\lambda_N \) evolves into a symmetric function \( \Psi^\lambda_N \).

Assume that the initial wave functions \( \Psi^\lambda_N \approx \prod_{j=1}^N \varphi^0(x_j) \) where \( \varphi^0 \in L^2(\mathbb{R}^3) \) and that the Gross-Pitaevskii equation

\[ i\dot{\varphi}^t = (-\Delta + A^t + a|\varphi^t|^2)\varphi^t \]  

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

Derivations of the Gross-Pitaevskii equation are usually based on a hierarchical method analogous to BBGKY hierarchies \([1, 2]\) where positivity of the interaction is assumed. 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 \( \mu^{\varphi_0} \) to a pure state \( |\varphi_0\rangle \langle \varphi_0| \). Furthermore we have to restrict the scaling behavior of the interaction to \( \beta < 1/6 \).

As it seems one needs these assumptions not only for technical reasons. Without positivity condition on the interaction there might be regimes where the Gross-Pitaevskii description breaks down: Assume for example that the unscaled interaction \( v \) is negative inside some ball of radius \( R \), but positive outside this ball such that the scattering length of the scaled potential is positive. The ground state energy of such a system tends to minus infinity as \( N \to \infty \): Put all particles in a box of diameter \( RN^{-1/3} \). The interaction energy per particle is then negative and of order \( N^{2/3} \) and dominates the kinetic energy per particle which grows like \( N^{1/3} \). One expects that the clustering of particles may also lead to a different dynamical behavior of the reduced density of the \( N \)-body problem and the solution of the Gross-Pitaevskii equation, nevertheless a rigorous treatment of that question has never been given.

Assuming a high purity of the initial condensate (i.e. fast convergence of \( \mu^{\varphi_0} \) to \( |\varphi_0\rangle \langle \varphi_0| \)) and moderate scaling behavior of the interaction clustering of the particles can be avoided and the Gross-Pitaevskii description stays valid.

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 \( \varphi^t \)) using the method presented in \([5]\). Following \([5]\) 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 1 Let \( \varphi \in L^2(\mathbb{R}^3) \).

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

\[ p_j^\varphi \Psi_N = \varphi(x_j) \int \varphi^*(x_j) \Psi_N(x_1, \ldots, x_N)d^3x_j \quad \forall \Psi_N \in L^2(\mathbb{R}^{3N}) \]
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 $0 \leq k \leq N$ we define the set

$$A_k := \{(a_1, a_2, \ldots, a_N) : a_k \in \{0, 1\}; \sum_{j=1}^N a_j = k\}$$

and the orthogonal projector $P_k^\varphi$ acting on $L^2(\mathbb{R}^3N)$ as

$$P_k^\varphi := \sum_{a \in A_k} \prod_{j=1}^N (p_j^\varphi)^{1-a_j}(q_j^\varphi)^{a_j}.$$

For negative $k$ and $k > N$ we set $P_k^\varphi := 0$.

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

$$\widehat{f}^\varphi := \sum_{j=0}^N f(j) P_j^\varphi. \quad (4)$$

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

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

**Notation 1** Throughout the paper hats $\widehat{\cdot}$ shall solemnly be used in the sense of Definition 1(c). The label $n$ shall always be used for the function $n(k) = \sqrt{k/N}$.

With Definition 1 we arrive directly at the following lemma based on combinatorics of the $p_j^\varphi$ and $q_j^\varphi$:

**Lemma 1**

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

$$\widehat{f}^\varphi g^\varphi = \widehat{g}^\varphi = g^\varphi \widehat{f}^\varphi \quad \widehat{f}^\varphi p_j^\varphi = p_j^\varphi \widehat{f}^\varphi \quad \widehat{f}^\varphi P_k^\varphi = P_k^\varphi \widehat{f}^\varphi.$$

(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 $\varphi$, i.e.

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

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

$$\| \widehat{f}^\varphi q_1^\varphi \Psi_N \|^2 = \| \widehat{f}^\varphi \widehat{n}^\varphi \Psi_N \|^2, \quad (5)$$

$$\| \widehat{f}^\varphi q_1^\varphi q_2^\varphi \Psi_N \|^2 \leq \frac{N}{N-1} \| \widehat{f}^\varphi (\widehat{n}^\varphi)^2 \Psi_N \|^2. \quad (6)$$
(d) For any function \( m : \{0, 1, \ldots, N\} \to \mathbb{R}_0^+ \), any function \( f : \mathbb{R}^6 \to \mathbb{R} \) and any \( j, k = 0, 1, 2 \) we have
\[
Q^\psi_k f(x_1, x_2) Q^\psi_j \hat{m}^\psi = Q^\psi_k \hat{m}^\psi_{j-k} f(x_1, x_2) Q^\psi_j,
\]
where \( Q^\psi_0 := p^\psi_1 p^\psi_2, Q^\psi_1 := p^\psi_1 q^\psi_2 + q^\psi_1 p^\psi_2 \) and \( Q^\psi_2 := q^\psi_1 q^\psi_2 \).

**Proof**

(a) follows immediately from Definition 1, using that \( p_j \) and \( q_j \) are orthogonal projectors.

(b) Note that \( \bigcup_{k=0}^N A_k = \{0, 1\}^N \), so \( 1 = \sum_{k=0}^N P^\psi_k \). Using also \( (q^\psi_k)^2 = q^\psi_k \) and \( q^\psi_k p^\psi_k = 0 \) we get
\[
N^{-1} \sum_{k=1}^N q^\psi_k = N^{-1} \sum_{k=1}^N q^\psi_k \sum_{j=0}^N P^\psi_j = N^{-1} \sum_{j=0}^N \sum_{k=1}^N q^\psi_k P^\psi_j = N^{-1} \sum_{j=0}^N j P^\psi_j
\]
and (b) follows.

(c) Let \( \langle \cdot, \cdot \rangle \) be the scalar product on \( L^2(\mathbb{R}^{3N}) \). For (5) we can write using symmetry of \( \Psi_N \)
\[
\| \hat{f}^\psi n^\psi \Psi_N \|^2 = \langle \Psi_N, (\hat{f}^\psi)^2 (n^\psi)^2 \Psi_N \rangle = N^{-1} \sum_{k=1}^N \langle \Psi_N, (\hat{f}^\psi)^2 q^\psi_k \Psi_N \rangle = \| \hat{f}^\psi q^\psi_1 \Psi_N \|^2.
\]
Similarly we have for (6)
\[
\| \hat{f}^\psi (n^\psi)^2 \Psi_N \|^2 = \langle \Psi_N, (\hat{f}^\psi)^2 (n^\psi)^4 \Psi_N \rangle = N^{-2} \sum_{j,k=1}^N \langle \Psi_N, (\hat{f}^\psi)^2 q^\psi_j q^\psi_k \Psi_N \rangle
\]
\[
= N^{-1} \langle \Psi_N, (\hat{f}^\psi)^2 q^\psi_1 q^\psi_2 \Psi_N \rangle + N^{-1} \langle \Psi_N, (\hat{f}^\psi)^2 q^\psi_1 q^\psi_2 \Psi_N \rangle
\]
\[
= N^{-1} \| \hat{f}^\psi q^\psi_1 q^\psi_2 \Psi_N \|^2 + N^{-1} \| \hat{f}^\psi q^\psi_1 \Psi_N \|^2,
\]
and (c) follows.

(d) Using the definitions above we have
\[
Q^\psi_k f(x_1, x_2) Q^\psi_j \hat{m}^\psi = \sum_{l=0}^N m(l) Q^\psi_k f(x_1, x_2) Q^\psi_j P^\psi_l.
\]
The number of projectors \( q^\psi_k \) in each term in the sum representing \( P^\psi_j Q^\psi_j \) in the coordinates \( k = 3, \ldots, N \) is equal to \( l - j \). The \( p^\psi_k \) and \( q^\psi_k \) with \( k = 3, \ldots, N \) commute with \( f(x_1, x_2) \) and with \( Q^\psi_j \). Thus \( Q^\psi_k f(x_1, x_2) Q^\psi_j P^\psi_l = P^\psi_{l-j+k} Q^\psi_k f(x_1, x_2) Q^\psi_j \) and
\[
Q^\psi_k f(x_1, x_2) Q^\psi_j \hat{m}^\psi = \sum_{l=0}^N m(l) P^\psi_{l-j+k} Q^\psi_k f(x_1, x_2) Q^\psi_j.
\]
\[
\sum_{l=k-j}^{N+k-j} m(l + j - k) P_l^Q f(x_1, x_2) Q_j^w
\]
\[
= \tilde{m}_{j-k}^Q f(x_1, x_2) Q_j^w.
\]

3 Derivation of the Gross-Pitaevskii Equation

As presented in [5] we wish to control the functional \( \alpha_N : L^2(\mathbb{R}^{3N}) \times L^2(\mathbb{R}^3) \to \mathbb{R}_0^+ \) given by

\[
\alpha_N(\Psi_N, \varphi) = \langle \Psi_N, \tilde{m}^\varphi \Psi_N \rangle
\]

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 2). For these weights convergence of the respective \( \alpha \) is stronger than \( \mu^\Psi_N \to |\varphi\rangle \langle \varphi| \) in operator norm (see Lemma 2).

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 2** 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 \( \alpha_N^\lambda : L^2(\mathbb{R}^{3N}) \times L^2(\mathbb{R}^3) \to \mathbb{R}_0^+ \) by

\[
\alpha_N^\lambda(\Psi_N, \varphi) := \langle \Psi_N, \tilde{m}^\varphi \Psi_N \rangle = \| (\tilde{m}^\varphi) \|^{1/2} \Psi_N \|^2.
\]

With these definitions we arrive at the main theorem:

**Theorem 1** Let \( 0 < \lambda, \beta < 1 \), let \( v_N^\beta(x) \) satisfy Assumption 1. Let \( A^t \) be a time dependent potential. Assume that for any \( N \in \mathbb{N} \) there exists a solution of the Schrödinger equation \( \Psi_N^t \) and a \( L^\infty \) solution of the Gross-Pitaevskii equation (3) \( \varphi^t \) on some interval \([0, T)\) with \( T \in \mathbb{R}^+ \cup \{ \infty \} \).

Then for any \( t \in [0, T) \)

\[
\alpha_N^\lambda(\Psi_N^t, \varphi^t) \leq e^{\int_0^t C_v \| \varphi^t \|^2 \| \Delta \| ds} \alpha_N^\lambda(\Psi_N^0, \varphi^0) + \left( e^{\int_0^t C_v \| \varphi^t \|^2 \| \Delta \| ds} - 1 \right) N^{\delta_\lambda} \sup_{0 \leq s \leq t} K^{\varphi^t},
\]

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

\[
K^{\varphi} := C_v \left( \| \Delta \varphi \|^2 + \| \varphi \|_\infty \right) \| \varphi \|_\infty.
\]

The proof of the theorem shall be given below.
Remark 1 For $\beta < 1/6$ one can choose $\lambda$ such that $\delta_3$ is negative: Choose $\lambda = 1 - 3\beta - \xi$ for some $\xi > 0$. Then $1 + \lambda + 3\beta = -\xi$ is negative. Furthermore $1 - \lambda - 4\beta = \xi - \beta$ and $3\beta - \lambda = \xi - 1 + 6\beta$ are negative for sufficiently small $\xi$.

3.1 Convergence of the Reduced Density Matrix

In [5] Lemma 2.2 it is shown that convergence of $\alpha_N(\Psi_N, \varphi) \to 0$ 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 $\alpha^\lambda_N(\Psi_N, \varphi) \geq \langle \Psi_N, (\hat{n}^{\varphi})^2 \Psi_N \rangle$ (recall that $n(k) = \sqrt{k/N}$). It follows with Lemma 2.2 in [5] that for all $0 < \lambda < 1$

$$\lim_{N \to \infty} \alpha^\lambda_N(\Psi_N, \varphi) = 0 \Rightarrow \lim_{N \to \infty} \mu^{\Psi_N} \to |\varphi\rangle \langle \varphi|$$

in operator norm.

Therefore our result implies convergence of the respective reduced one particle marginal density. To be able to formulate Theorem 1 under conditions of the reduced one particle marginal density we have the following lemma

Lemma 2 Let $0 < \lambda < 1$, $\xi < 0$ and let $\|\mu^\Psi - |\varphi\rangle \langle \varphi|\|_\text{op} = O(N^{\xi})$. Then

$$\alpha^\lambda_N(\Psi_N, \varphi) = O(N^{1-\lambda+\xi}).$$

Proof Under the assumptions $\|\mu^\Psi - |\varphi\rangle \langle \varphi|\|_\text{op} = O(N^{\xi})$ it follows that

$$\|p_1^\varphi \Psi_N\|^2 = \langle \Psi_N, p_1^\varphi \Psi_N \rangle = \text{tr} p_1^\varphi \mu^\Psi = \langle \varphi, \mu^\Psi \varphi \rangle = 1 + \langle \varphi, (\mu^\Psi - |\varphi\rangle \langle \varphi|) \varphi \rangle \leq 1 + O(N^{\xi}).$$

Using that $p_1^\varphi$ and $q_1^\varphi$ are orthogonal projectors and Lemma 1(c)

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

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

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

As already explained this lemma allows us to formulate the theorem under conditions of the reduced density matrix. With Lemma 2.2 of [5] (i.e. Lemma 2.3. of [4]) we can also formulate the result in terms of $\mu^\Psi$.

Corollary 1 Let $0 < \lambda, \beta < 1$ be such that $1 - \lambda - 4\beta$, $3\beta - \lambda$ and $-1 + \lambda + 3\beta$ are negative. Let $\psi_N^0(\xi)$ satisfy Assumption 1. Let $A'$ be a time dependent potential. Assume that for any $N \in \mathbb{N}$ there exists a solution of the Schrödinger equation $\Psi_N^0$ and a $L^\infty$ solution of the Gross-Pitaevskii equation (3) $\psi'$ on some interval $[0, T)$ with $T \in \mathbb{R}^+ \cup \{\infty\}$ such that $\int_0^T \|\psi'|^2 \Delta ds + \sup_{0 \leq s < T} (\|\Delta |\varphi|^2\| + \|\varphi\|_{\infty})$ are finite. Let $\|\mu^\Psi - |\varphi^0\rangle \langle \varphi^0|\|_\text{op} = O(N^{\lambda-1})$. Then

$$\lim_{N \to \infty} \|\mu^\Psi - |\varphi'|\langle \varphi'|\|_\text{op} = 0$$

uniform in $0 \leq t < T$. 

\[ \text{Springer} \]
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 $f : L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N})$ by

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

In particular we shall need the following proposition

**Proposition 1**

(a) For any $f \in L^2(\mathbb{R}^3)$

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

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

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

**Proof**

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

$$\| f(x_1) p_1^\psi \|_{op}^2 = \sup_{\| \Psi_N \| = 1} \langle \Psi_N, p_1^\psi f^2(x_1) p_1^\psi \Psi_N \rangle$$

$$= \sup_{\| \Psi_N \| = 1} \langle \Psi_N, \varphi(x_1) \varphi(x_1) \rangle \langle f^2(x_1) \varphi(x_1) \varphi(x_1) \rangle \langle \Psi_N \rangle$$

$$= \langle \varphi(x_1) \rangle^2 \langle f^2(x_1) \varphi(x_1) \rangle \sup_{\| \Psi_N \| = 1} \langle \Psi_N, \varphi(x_1) \varphi(x_1) \rangle \langle \Psi_N \rangle$$

$$= \langle \varphi(x_1) \rangle^2 \langle f^2(x_1) \varphi(x_1) \rangle$$

Using Hölder the first factor is bounded by $\| f \|^2 \| \varphi \|_\infty^2$. Since $p_1^\psi$ is a projector the second factor equals one and (a) follows.

(b) Again writing $p_1^\psi = \varphi(x_1) \langle \varphi(x_1) \rangle$

$$\| f(x_1 - x_2) p_1^\psi \|_{op}^2 = \sup_{\| \Psi_N \| = 1} \| f(x_1 - x_2) p_1^\psi \Psi_N \|^2$$

$$= \sup_{\| \Psi_N \| = 1} \langle \Psi_N, \varphi(x_1) \varphi(x_1) \rangle \langle f(x_1 - x_2)^2 \varphi(x_1) \varphi(x_1) \rangle \langle \Psi_N \rangle.$$

Using that

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

one gets

$$\| f(x_1 - x_2) p_1^\psi \|_{op}^2 \leq \sup_{\| \Psi_N \| = 1} \| \Psi_N \|^2 \| \varphi \|_\infty^2 \| f \|^2 = \| \varphi \|_\infty^2 \| f \|^2.$$
(c) Let \( g \in L^1(\mathbb{R}^3) \).
\[
\| p_1^g g(x_1 - x_2) p_1^g \|_{op} \leq \| p_1^g |g(x_1 - x_2)| p_1^g \|_{op} = \| p_1^g \sqrt{|g(x_1 - x_2)|} \|_{op} \leq \| \sqrt{|g(x_1 - x_2)|} p_1^g \|_{op}^2.
\]

With (b) we get (c). \( \square \)

We shall prove the theorem using a Grönwall argument. The idea behind the Grönwall argument is as follows: Assume one wants to show that some positive time dependent value—let us say \( \eta' \)—is small for \( t > 0 \) knowing it was small at time \( t = 0 \). This can be achieved by showing that the time derivative of \( \eta' \) is small for all times \( 0 < s < t \). Following Grönwall’s idea it is enough to control \( \dot{\eta}' \) in terms of \( \eta' \) itself and some other small value \( \varepsilon \): Assuming \( \dot{\eta}' \leq C t (\eta' + \varepsilon) \) one gets that \( \eta' \) is bounded by the solution \( \zeta' \) of
\[
\dot{\zeta}' = C (\zeta' + \varepsilon).
\]
The solution of this differential equation is
\[
\zeta' = e^{\int_0^t C s ds} \eta' + \left( e^{\int_0^t C s ds} - 1 \right) \varepsilon.
\]
To get the estimates as stated in Theorem 1 it is sufficient to show that
\[
|\dot{\alpha}^\lambda_N(\Psi^t_N, \varphi')| \leq C_v \|\varphi'\|_{\infty}^2 \alpha^\lambda_N(\Psi^t_N, \varphi') + K_{\varphi'} N^\delta.
\]
(7)

To shorten notation we use the following definitions:

**Definition 3** 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 \( \gamma^\lambda_N : L^2(\mathbb{R}^3N) \times L^2(\mathbb{R}^3) \rightarrow \mathbb{R} \) by
\[
\gamma^\lambda_N(\Psi^t_N, \varphi) = 2 \Im \left( \langle \Psi^t_N, (\tilde{m}^\lambda_\varphi - \tilde{m}^\lambda_\varphi) p_1 q_2 h_{1,2} p_1 p_2 \Psi_N \rangle \right)
+ \Im \left( \langle \Psi^t_N, (\tilde{m}^\lambda_\varphi - \tilde{m}^\lambda_\varphi) q_1 q_2 h_{1,2} p_1 p_2 \Psi_N \rangle \right)
+ 2 \Im \left( \langle \Psi^t_N, (\tilde{m}^\lambda_\varphi - \tilde{m}^\lambda_\varphi) q_1 q_2 h_{1,2} p_1 p_2 \Psi_N \rangle \right).
\]

\( \gamma^\lambda_N \) was defined in such a way that for any solution of the Schrödinger equation \( \Psi^t_N \) and any solution \( \varphi' \) of the Gross-Pitaevskii equation \( \dot{\alpha}^\lambda_N(\Psi^t_N, \varphi') = \gamma^\lambda_N(\Psi^t_N, \varphi') \) (see Lemma 3 below). It is left to show that \( \gamma^\lambda_N(\Psi_N^t, \varphi') \) can be controlled by \( \alpha^\lambda_N(\Psi^t_N, \varphi') \) and \( N^{-\delta} \) (which is done in Lemma 4 below) to get (7) and—via Grönwall—the theorem.
Lemma 3 For any solution of the Schrödinger equation $\Psi_N^t$, any solution of the Gross-Pitaevskii equation $\varphi^t$ and any $0 < \lambda < 1$ we have

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

Proof Let

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

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

$$\frac{d}{dt} \tilde{\gamma}^t = i[H_{GP}^{\varphi}, \tilde{\gamma}^t]$$

for any weight $r : \{0, \ldots, N\} \to \mathbb{R}$. With (8) we get

$$\dot{\alpha}_N(\Psi_N^t, \varphi^t) = i\langle \Psi_N^t, \hat{m}_\lambda^{\varphi} H \Psi_N^t \rangle - i\langle H \Psi_N^t, \hat{m}_\lambda^{\varphi} \Psi_N^t \rangle$$

$$+ i\langle \Psi_N^t, [H_{GP}^{\varphi}, \hat{m}_\lambda^{\varphi}] \Psi_N^t \rangle$$

$$= -i\langle \Psi_N^t, [H - H_{GP}^{\varphi}, \hat{m}_\lambda^{\varphi}] \Psi_N^t \rangle.$$

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

$$\dot{\alpha}_N(\Psi_N^t, \varphi^t) = -i(N^2 - N)^{-1} \sum_{1 \leq j < k \leq N} \langle \Psi_N^t, [h_{j,k}, \hat{m}^{\varphi}] \Psi_N^t \rangle$$

$$= -i\langle \Psi_N^t, [h_{1,2}, \hat{m}^{\varphi}] \Psi_N^t \rangle / 2.$$

Let us next establish a formula for the commutator. Remember the notation $Q_0^\varphi := p_1 p_2^\varphi$, $Q_1^\varphi := p_1^\varphi q_2 + q_1^\varphi p_2$ and $Q_2^\varphi := q_1^\varphi q_2^\varphi$ from Lemma 1(d) and that $\sum_{k=0}^{2} Q_k^\varphi = 1$. For any function $f : \mathbb{R}^2 \to \mathbb{R}$, any $\varphi \in L^2$ and any weight $r : \{0, \ldots, N\} \to \mathbb{R}$

$$[f(x_1, x_2), \tilde{\gamma}^t] = \sum_{k=0}^{2} Q_k^\varphi f(x_1, x_2) \tilde{\gamma}^t Q_k^\varphi - \sum_{k=0}^{2} Q_k^\varphi \tilde{\gamma}^t f(x_1, x_2) Q_k^\varphi$$

Lemma 1(d) gives

$$[f(x_1, x_2), \tilde{\gamma}^t] = \sum_k (\tilde{\gamma}^t - \tilde{\gamma}^t) Q_k^\varphi f(x_1, x_2) Q_k^\varphi$$

$$+ \sum_{k < j} (\tilde{\gamma}_{j-k}^t - \tilde{\gamma}^t) Q_k^\varphi f(x_1, x_2) Q_j^\varphi$$

$$+ \sum_{k > j} Q_k^\varphi f(x_1, x_2) Q_j^\varphi (\tilde{\gamma}^t - \tilde{\gamma}_{k-j}^t).$$

The first summand is zero, the third is the adjoint of the second. Thus setting $r = m^\lambda$ and $f(x_1, x_2) = h_{1,2}$ we get with (9)

$$\dot{\alpha}_N(\Psi_N^t, \varphi^t) = \sum_{k < j} \Im \left( \langle \Psi_N^t, (\hat{m}_{j-k}^{\varphi} - \hat{m}^{\varphi}) Q_k^\varphi h_{1,2} Q_j^\varphi, \Psi_N^t \rangle \right).$$
Using symmetry (recall that \( Q_\nu^\rho = p_1^\rho q_2^\rho + q_1^\rho p_2^\rho \), thus it can due to symmetry be replaced by \( 2p_1^\rho q_2^\rho \)) the lemma follows. \( \square \)

With Lemma 3 (7) follows once we can control the different summands appearing in \( \gamma_N^\lambda \) in a suitable way. So the following lemma completes the proof of the theorem.

**Lemma 4** Let \( v_N^\rho \) satisfy Assumption 1. Then there exists a \( C < \infty \) such that for any \( \varphi \in L^\infty \) with \( \Delta |\varphi|^2 \in L^2 \)

(a) \[
\left| \langle \Psi_N, (\hat{m}_{-1}^\lambda - \hat{m}^\lambda) p_1^\rho q_2^\rho h_{1,2} p_1^\rho p_2^\rho \Psi_N \rangle \right| \leq K^\rho N^{\delta_\lambda}.
\]

(b) \[
\left| \langle \Psi_N, (\hat{m}_{-1}^\lambda - \hat{m}^\lambda) q_1^\rho q_2^\rho h_{1,2} p_1^\rho p_2^\rho \Psi_N \rangle \right| \leq C \|v\|_\infty^2 \alpha_N^\rho (\Psi_N, \varphi) + K^\rho N^{\delta_\lambda}.
\]

(c) \[
\left| \langle \Psi_N, (\hat{m}_{-1}^\lambda - \hat{m}^\lambda) q_1^\rho q_2^\rho h_{1,2} p_1^\rho q_2^\rho \Psi_N \rangle \right| \leq K^\rho N^{\delta_\lambda}
\]

with \( \delta_\lambda \) and \( K^\rho \) as in Theorem 1.

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 \( p_1^\rho q_2^\rho h_{1,2} p_1^\rho p_2^\rho \) is small.

For (c) the choice of the weights \( m^\lambda \) plays an important role. Note that we only have one projector \( p^\rho \) here and \( \|q_1^\rho q_2^\rho h_{1,2} p_1^\rho \|_{op} \) can not be controlled by the \( L^1 \)-norm of \( v \) (see Proposition 1). On the other hand we have altogether three projectors \( q^\rho \) in (c). Using Lemma 1(c) we will see that these projectors \( q_1^\rho \) in combination with the operator \( (\hat{m}_{-1}^\lambda - \hat{m}^\lambda) \) make this term small: The operator norm of \( (\hat{m}^\lambda)^3 (\hat{m}_{-1}^\lambda - \hat{m}^\lambda) \) is of order \( N^{-(3+\lambda)/2} \).

**Proof** In the proof we shall drop the indices \( \lambda, N \) and \( \varphi \) 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.

We will also use that the scaling of \( v_N^\rho \) is such that \( \|v_N^\rho\|_1 = a/N \) and \( \|v_N^\rho\| \leq C N^{-1+3/\beta} \).

(a) In bra-ket notation \( p_1 = |\varphi(x_1)\rangle \langle \varphi(x_1)| \). Writing \( \star \) for the convolution we get for any \( f : \mathbb{R}^3 \to \mathbb{R} \)

\[
p_1 f(x_1 - x_2) p_1 = |\varphi(x_1)\rangle \langle \varphi(x_1)| f(x_1 - x_2)|\varphi(x_1)\rangle \langle \varphi(x_1)|
\]

\[
= p_1 (f \star |\varphi|^2)(x_2), \quad (10)
\]

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

\[
p_1 q_2 h_{1,2} p_1 p_2 = N p_1 q_2 \left( (N - 1) u_N^\rho(x_1 - x_2) - a |\varphi|^2(x_2) \right) p_1 p_2
\]

\[
= N p_1 q_2 \left( (N - 1) u_N^\rho(x_1 - x_2) - a \delta(x_1 - x_2) \right) p_1 p_2.
\]
Using this and triangle inequality the left hand side of (a) is bounded by
\[
N|\langle \Psi, (\hat{m} - \hat{m}) p_1 q_2 (N v_N^\beta (x_1 - x_2) - a \delta (x_1 - x_2)) p_1 p_2 \Psi \rangle| \\
+ N|\langle \Psi, (\hat{m} - \hat{m}) p_1 q_2 v_N^\beta (x_1 - x_2) p_1 p_2 \Psi \rangle|.
\]  
(11)

To control the first summand we define the function \(f_N^\beta : \mathbb{R}^3 \rightarrow \mathbb{R}\) by
\[
\Delta f_N^\beta = N v_N^\beta - a \delta.
\]

Recall that \(v\) is compactly supported. Since \(N \int v(x) d^3 x = a\) the integration constant of \(f_N^\beta\) can be chosen such that also \(f_N^\beta\) has compact support. Using the scaling behavior of \(v_N^\beta\) it follows that
\[
f_N^\beta = N^\beta f(N^\beta x) \quad \text{and} \quad \|f_N^\beta\|_1 = N^{-2\beta} \|f\|_1.
\]

Now we can estimate the first summand in (11) using (10)
\[
N|\langle \Psi, (\hat{m} - \hat{m}) p_1 q_2 \Delta f_N^\beta (x_1 - x_2) p_1 p_2 \Psi \rangle| \\
= N|\langle \Psi, (\hat{m} - \hat{m}) p_1 q_2 ((\Delta f_N^\beta) \ast |\varphi|^2)(x_2) p_1 p_2 \Psi \rangle| \\
= N|\langle \Psi, (\hat{m} - \hat{m}) p_1 q_2 (f_N^\beta \ast (\Delta |\varphi|^2))(x_2) p_1 p_2 \Psi \rangle|.
\]

Since \(\|p_1 p_2 \Psi\| \leq 1\) one gets with Proposition 1(a)
\[
\leq N\|(\hat{m} - \hat{m}) q_2 \Psi\| \| f_N^\beta \ast (\Delta |\varphi|^2)(x_2) p_2\|_{op} \\
\leq N\|(\hat{m} - \hat{m}) q_2 \Psi\| \| f_N^\beta \ast (\Delta |\varphi|^2)\| \|\varphi\|_\infty.
\]

In view of Lemma 1(b) we have using symmetry of \(\Psi\) for the first factor
\[
\|(\hat{m} - \hat{m}) q_2 \Psi\| = \|(\hat{m} - \hat{m}) n_2 \Psi\| \\
\leq \sup_{0 \leq k \leq N^\lambda} \left( \left| \frac{k - 1}{N^\lambda} - \frac{k}{N^\lambda} \right| \sqrt{k/N} \right) = (N^\lambda N)^{-1/2}.
\]  
(12)

Using Young’s inequality we have for the second factor
\[
\| f_N^\beta \ast (\Delta |\varphi|^2)\| \leq \| f_N^\beta\|_1 \|\Delta |\varphi|^2\| \leq C N^{-2\beta} \|\Delta |\varphi|^2\|.
\]

It follows that the first summand of (11) is bounded by
\[
C \|\Delta |\varphi|^2\| \|\varphi\|_\infty N^{(1 - \lambda - 4\beta)/2}. 
\]  
(13)

Using Schwarz inequality, then Proposition 1(c) and (12) the second summand of (11) is smaller than
\[
N\|(\hat{m} - \hat{m}) q_2 \Psi\| \| p_1 v_N^\beta (x_1 - x_2) p_1\|_{op} \\
\leq N\|(\hat{m} - \hat{m}) q_2 \Psi\| \| v_N^\beta\|_1 \|\varphi\|_\infty^2 \leq C (N^\lambda N)^{-1/2} \|\varphi\|_\infty^2.
\]
We use first that $q_1 q_2 w(x_1) p_1 p_2 = 0$ for any function $w$. It follows with Lemma 1(d) that

$$\langle \Psi, (m - \hat{m})^2 q_1 q_2 h_{1,2} p_1 p_2 \Psi \rangle = (N^2 - N) \langle \Psi, q_1 q_2 (\hat{m} - \hat{m})^{1/2} v_N^\beta (x_1 - x_2) (\hat{m} - \hat{m})^{1/2} p_1 p_2 \Psi \rangle. \quad (14)$$

Before we estimate this term note that the operator norm of $q_1 q_2 v_N^\beta (x_1 - x_2)$ restricted to the subspace of symmetric functions is much smaller than the operator norm on full $L^2(\mathbb{R}^3)$. This comes from the fact that $v_N^\beta (x_1 - x_2)$ 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 (14) 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 that (14) equals

$$(N^2 - N) \langle \Psi, q_1 q_2 (\hat{m} - \hat{m})^{1/2} v_N^\beta (x_1 - x_2) (\hat{m} - \hat{m})^{1/2} p_1 p_2 \Psi \rangle$$

$$= N \left\| \langle \Psi, (\hat{m} - \hat{m})^{1/2} \sum_{j=2}^N q_1 q_j v_N^\beta (x_1 - x_j) p_1 p_j (\hat{m} - \hat{m})^{1/2} \Psi \rangle \right\| \leq N \| (\hat{m} - \hat{m})^{1/2} q_1 \Psi \| \left\| \sum_{j=2}^N q_j v_N^\beta (x_1 - x_j) p_1 p_j (\hat{m} - \hat{m})^{1/2} \Psi \right\|.$$

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

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

The square of the second factor is bounded by

$$\sum_{2 \leq j < k \leq N} \langle (\hat{m} - \hat{m})^{1/2} \Psi, p_1 p_j v_N^\beta (x_1 - x_j) q_j q_k v_N^\beta (x_1 - x_k) (\hat{m} - \hat{m})^{1/2} p_1 p_k \Psi \rangle$$

$$+ \sum_{k=2}^N \| q_k v_N^\beta (x_1 - x_k) p_1 p_k (\hat{m} - \hat{m})^{1/2} \Psi \|^2. \quad (15)$$

Using symmetry and Proposition 1(b) the first summand in (15) is bounded by

$$N^2 \langle (\hat{m} - \hat{m})^{1/2} \Psi, p_1 p_2 q_3 v_N^\beta (x_1 - x_2) v_N^\beta (x_1 - x_3) p_1 q_2 p_3 (\hat{m} - \hat{m})^{1/2} \Psi \rangle$$

$$\leq N^2 \| v_N^\beta (x_1 - x_2) \| v_N^\beta (x_1 - x_3) \| p_1 q_2 p_3 (\hat{m} - \hat{m})^{1/2} \Psi \|^2$$

$$\leq N^2 \| v_N^\beta (x_1 - x_2) \| \| p_1 \|_o^4 \| (\hat{m} - \hat{m})^{1/2} q_2 \Psi \|^2$$

$$\leq N^2 \| \varphi \|_{\infty}^4 \| v_N^\beta \|_1^2 \| (\hat{m} - \hat{m})^{1/2} q_2 \Psi \|^2$$

$$\leq CN^{-1} \| \varphi \|_{\infty}^4 \alpha_N (\Psi, \varphi).$$
Using Proposition 1(c) the second summand in (15) can be controlled by

\[ N \langle (\hat{m} - \hat{m}_2)^{1/2} \Psi, p_1 p_2 (v^\beta_N (x_1 - x_2))^2 p_1 p_2 (\hat{m} - \hat{m}_2)^{1/2} \Psi \rangle \]

\[ \leq N \| p_1 (v^\beta_N (x_1 - x_2))^2 p_1 \|_\text{op} \| (\hat{m} - \hat{m}_2)^{1/2} \|_\text{op}^2 \]

\[ \leq N \| \varphi \|_\infty^2 \| v^\beta_N \|_2^2 \| (\hat{m} - \hat{m}_2)^{1/2} \|_\text{op}^2 \leq C \| \varphi \|_\infty^2 N N^{-2+3\beta} N^{-\lambda}. \]

It follows that (15) is bounded by

\[ CN^{-1} \| \varphi \|_\infty^2 (\| \varphi \|_\infty^2 \alpha_N (\Psi, \varphi) + CN^{-\lambda+3\beta}), \]

thus (14) is bounded by

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

(c) Using Lemma 1(d) and Cauchy-Schwarz we get for the left hand side of (c)

\[ \left| \langle \Psi, (\hat{m} - \hat{m})\hat{n}_1 q_1 q_2 h_{1,2} \hat{n}^{-1} p_1 q_2 \Psi \rangle \right| \]

\[ \leq \| (\hat{m} - \hat{m})\hat{n}_1 q_1 q_2 \| \| h_{1,2} \hat{n}^{-1} p_1 q_2 \| \| \Psi \|. \]

For the first factor we have using Lemma 1(c)

\[ \| (\hat{m} - \hat{m})\hat{n}_1 q_1 q_2 \| \leq \frac{N}{N - 1} \| (\hat{m} - \hat{m})\hat{n}_1 \hat{n}_2 \| \]

\[ \leq \sup_{0 < k < N^\lambda} \left( \frac{N}{N - 1} \left| \frac{k - 1}{N^\lambda} - \frac{k}{N^\lambda} \right| (k/N)^{3/2} \right) \]

\[ = \frac{N^{(\lambda-1)/2}}{N - 1}. \]

For the second factor we have using Lemma 1(c), triangle inequality and Proposition 1(b)

\[ \| h_{1,2} \hat{n}^{-1} p_1 q_2 \| \leq \| h_{1,2} p_1 \|_\text{op} \| \hat{n}^{-1} q_2 \| = \| h_{1,2} p_1 \|_\text{op} \]

\[ \leq N (N - 1) \| v^\beta_N (x_1 - x_2) \| p_1 \|_\text{op} \]

\[ + N \| a | \varphi(x_1) \|_2 | p_1 \|_\text{op} + N \| a | \varphi(x_2) \|_2^2 | p_1 \|_\text{op} \]

\[ \leq N (N - 1) \| \varphi \|_\infty \| v^\beta_N \| + 2a N \| \varphi \|_\infty^2 \]

\[ \leq CN \| \varphi \|_\infty^2 (N - 1) N^{-1+3/2\beta} + \| \varphi \|_\infty^2 \].

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

\[ CN \frac{N^{(\lambda-1)/2}}{N - 1} (N - 1) N^{-1+3/2\beta} (\| \varphi \|_\infty + \| \varphi \|_\infty^2) \]

\[ \leq C (\| \varphi \|_\infty^2 + \| \varphi \|_\infty^2) N^{(\lambda-1+3\beta)/2}. \]
References

1. Erdös, L., Schlein, B., Yau, H.-T.: Derivation of the Gross-Pitaevskii hierarchy for the dynamics of Bose-Einstein condensate. Commun. Pure Appl. Math. 59(12), 1659–1741 (2006)
2. Erdös, L., Schlein, B., Yau, H.-T.: Derivation of the cubic non-linear Schrödinger equation from quantum dynamics of many-body systems. Invent. Math. 167, 515–614 (2007)
3. Ginibre, J., Ozawa, T.: Long range scattering for nonlinear Schrödinger and Hartree equations in space dimension \( n \geq 2 \). Commun. Math. Phys. 151(3), 619–645 (1993)
4. Knowles, A., Pickl, P.: Mean-field dynamics: singular potentials and rate of convergence. Commun. Math. Phys. (2010). doi:10.1007/s00220-010-1010-2
5. Pickl, P.: A simple derivation of mean field limits for quantum systems (2010)