On the Time Dependent Gross Pitaevskii- and Hartree Equation

P. Pickl *

May 29, 2018

Abstract

We are interested in solutions Ψ_t of the Schrödinger equation of N interacting bosons under the influence of a time dependent external field, where the range and the coupling constant of the interaction scale with N in such a way, that the interaction energy per particle stays more or less constant. Let $\mathcal{N}^{\varphi_0}$ be the particle number operator with respect to some $\varphi_0 \in L^2(\mathbb{R}^3 \to \mathbb{C})$. Assume that the relative particle number of the initial wave function $N^{-1}\langle\Psi_0, \mathcal{N}^{\varphi_0}\Psi_0\rangle$ converges to one as $N \to \infty$. We shall show that we can find a $\varphi_t \in L^2(\mathbb{R}^3 \to \mathbb{C})$ such that $\lim_{N\to\infty} N^{-1}\langle\Psi_t, \mathcal{N}^{\varphi_t}\Psi_t\rangle = 1$ and that φ_t is — dependent of the scaling of the range of the interaction — solution of the Gross-Pitaevskii or Hartree equation.

We shall also show that under additional decay conditions of φ_t the limit can be taken uniform in $t < \infty$ and that convergence of the relative particle number implies convergence of the k-particle density matrices of Ψ_t.

1 Introduction

In this paper we wish to analyze the dynamics of a Bose condensate of N interacting particles when the external trap — described by an external potential A_t — is changed, for example removed.

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

$$i\frac{d}{dt}\Psi_t = H\Psi_t \tag{1}$$

with some symmetric Ψ_0 we shall specify below and the Hamiltonian

$$H = -\sum_{j=1}^{N}\Delta_j + \sum_{j\neq k=1}^{n} v_\beta^N(x_j - x_k) + \sum_{j=1}^{N} A_t(x_j) \tag{2}$$

*Mathematisches Institut der Universität München, Theresienstr. 39, 80333 München, E-mail: pickl@mathematik.uni-muenchen.de

acting on the Hilbert space $L^2(\mathbb{R}^{3N} \to \mathbb{C})$, where $\beta \in \mathbb{R}$ stands for the scaling behavior of the interaction. The v_β^N we wish to analyze scales with the particle number in such a way, that the total interaction energy scales in the same way as the total kinetic energy of the N particles. For the heuristic arguments we shall give first one should think of a interaction which is given by $v_\beta^N(x) = N^{-1+3\beta}v(N^\beta x)$ for a compactly supported, spherically symmetric, positive potential $v \in L^\infty$. The interactions we shall choose below will be of a more general form. The A_t describing the trap potential is a time dependent external potential which we shall choose — in contrast to v_β^N — not N-dependent. Note, that H conserves symmetry, i.e. for any symmetric function Ψ_0 also $H\Psi_0$ and thus Ψ_t is symmetric.

Assume moreover that the initial wave function Ψ_0 is a condensate, i.e. that there exists a L^2 function φ_0 such that

$$\lim_{N\to\infty} \langle \Psi_0, \widehat{n}^{\varphi_0} \Psi_0 \rangle = 1$$

where $\widehat{n}^{\varphi_0}$ is the particle number operator of particles in φ_0 (see Definition 2.1 (c) and Lemma 2.3 (a)).

Under these and some additional technical assumptions we shall show that also Ψ_t will be a condensate, i.e. that there exist L^2 functions φ_t such that

$$\lim_{N\to\infty} \langle \Psi_0, \widehat{n}^{\varphi_t} \Psi_0 \rangle = 1$$

uniform in t on any compact subset of $\mathbb{R}^+$ and — under additional decay conditions on φ_t — uniform in $t \in \mathbb{R}^+$.

Even more: We shall show that φ_t solves the differential equation

$$i\frac{d}{dt}\varphi_t = -\left(\Delta + A_t + V_{\varphi_t}\right)\varphi_t \tag{3}$$

with φ_0 as above, where the "mean field" V_{φ_t} depends on φ_t itself, so (3) is a non-linear equation. For different regimes of β different effective mean field potentials will appear:

$\beta < 0$	$\beta = 0$	$0 < \beta \leq 1$	$\beta > 1$
$V_{\varphi_t} = 0$	$V_{\varphi_t} = v \star \lvert\varphi_t\rvert^2$	$V_{\varphi_t} = 2a\lvert\varphi_t\rvert^2$	$V_{\varphi_t} = 0$

We explain the table. For $\beta < 0$ $\lim_{N\to\infty} \left\| \sum_{j=2}^N v_\beta^N(x_1 - x_j) \right\|_\infty = 0$, so it is heuristically clear that the mean field is zero.

$v_0^N = v/N$ and hence particle (say number one) feels $N^{-1}\sum_{j=2}^N v(x_1 - x_j) \approx \int v(x-y)|\varphi_t|^2(y)d^3y$ assuming that the particles are $|\varphi_t|^2$-distributed. In this case (3) is called "Hartree equation". This limit has already been proven in the literature [8]. A sketch of an alternative proof shall be given below to motivate the technique used in this paper for the cases $0 < \beta \leq 1$ we shall focus on here.

For $0 < \beta$ the interaction becomes δ-like. To be able to "average out" the potential it is important to control the microscopic structure of Ψ_t. Assuming that the energy of Ψ_t is small, the microscopic structure is — whenever two particles approach — roughly given by the zero energy scattering length of the potential $1/2v_\beta^N$ (the factor $1/2$ comes from the fact that one has to go to relative coordinates of the two particles).

For $\beta = 1$ the scaling of the potential is such that the zero energy scattering state of $f^N(x)$ of the potential $v_\beta^N/2$ scales like $f^N = f_1(Nx)$. It follows that the mean field is given by $2a|\varphi_t|^2$, where a is the scattering length of $v/2$.

For $0 < \beta < 1$ the scaling is "softer" and the microscopic structure disappears as $N \to \infty$. Thus the mean field is given by $V_{\varphi_t} = \|v\|_1 |\varphi_t|^2$. One can also argue, that for "soft scalings" the scattering length is in good approximation given by the first order Born approximation, i.e. by the L_1-norm of the interaction.

For $\beta > 1$ note, that the scattering length of a spherically symmetric potential is always smaller than the radius of its support, thus for $\beta > 1$ $Na_N \to 0$ for $N \to \infty$, implying that the interaction becomes negligible for $\beta > 1$ as $N \to \infty$.

The cases $\beta = 1$ and $0 < \beta < 1$ have been proven recently for the special case $A_t \equiv 0$ [1, 2, 3, 4]. We shall give an alternative proof including time dependent external potentials and with weaker conditions on Ψ_0 and also generalizing to hard core potentials for $\beta = 1$.

2 Definition of the Projectors

Before we consider the different cases of $0 \le \beta \le 1$ we define the following operators acting on $L^2(\mathbb{R}^{3N} \to \mathbb{C})$ we shall need in the proofs below

Definition 2.1 *For any $\varphi \in L^2(\mathbb{R}^3 \to \mathbb{C})$ we define*

(a) for any $1 \le j \le N$ and any $\varphi \in L^2(\mathbb{R}^3 \to \mathbb{C})$ the orthogonal projector p_j^φ of the j^{th} particle onto φ defined by

$$p_j^\varphi \Psi := \varphi(x_j) \int \varphi(x_j)^* \Psi(x_1, \dots, x_N) d^3 x_j$$

for any $\Psi \in L^2(\mathbb{R}^{3N} \to \mathbb{C})$. We shall also need $q_j^\varphi = 1 - p_j^\varphi$.

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

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

For any $0 \le k \le j \le N$ and any $\varphi(x_j) \in L^2(\mathbb{R}^3 \to \mathbb{C})$ we define the orthogonal projector $P_{j,k}^\varphi$ acting on $L^2(\mathbb{R}^{3N} \to \mathbb{C})$ as

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

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

(c) *For any function* $f:\{0,1,\ldots,N\}\to\mathbb{R}^+$ *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*

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

We shall also need translations of the operators $\widehat{f}$*: Let* $f:\{0,1,\ldots,N\}\to\mathbb{R}^+$ *and* $d\in\mathbb{Z}$*. We define the operator* $\widehat{f}_d^\varphi : L^2(\mathbb{R}^{3N}\to\mathbb{C})\to L^2(\mathbb{R}^{3N}\to\mathbb{C})$ *as*

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

Notation 2.2 *Throughout the paper hats* $\widehat{\cdot}$ *shall solemnly be used in the sense of Definition 2.1 (c). In what follows the letter* C *will be used for various constants that need not be identical even within the same equation.*

With Definition 2.1 we arrive directly at the following Lemma based on combinatorics of the p_j^φ and q_j^φ:

Lemma 2.3 (a) *For any functions* $f,g\{0,1,\ldots,N\}\to\mathbb{R}^+$ *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* $n:\{0,1,\ldots,N\}\to\mathbb{R}^+$ *be given by* $n(k):=\sqrt{k/N}$*. Then the respective* $(\widehat{n}^\varphi)^2$ *(c.f. (4)) equals the relative particle number operator of particles not in the state* φ*, i.e.*

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

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

$$\left\|\widehat{f}^\varphi q_1^\varphi \Psi\right\|^2 = \|\widehat{f}^\varphi \widehat{n}^\varphi \Psi\|^2 \tag{5}$$

$$\left\|\widehat{f}^\varphi q_1^\varphi q_2^\varphi \Psi\right\|^2 \leq \frac{N}{N-1}\|\widehat{f}^\varphi (\widehat{n}^\varphi)^2 \Psi\|^2 \tag{6}$$

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

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

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

(e) For any $w \in L^\infty(\mathbb{R}^3 \to \mathbb{C})$ and any symmetric $\Psi \in L^2(\mathbb{R}^{3N} \to \mathbb{C})$

$$|\langle \Psi, w(x_1)\Psi\rangle - \langle \varphi, w\varphi\rangle| \leq 4\|w\|_\infty \left(N^{-1/4} + \|(\widehat{n}^\varphi)^{1/2}\Psi\|^2 \right) . \qquad (7)$$

Proof: (a) follows immediate from definition 2.1, using that p_j and q_j are orthogonal projectors.

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

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

and (b) follows.

For (5) we can write using symmetry of Ψ

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

Similarly we have for (6)

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

and (c) follows.

Using the definitions above we have for (d)

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

For (e) we have

$$\begin{aligned}|\langle \Psi, w(x_1)\Psi\rangle - \langle \varphi, w\varphi\rangle| &= \big|\langle p_1^\varphi \Psi, w(x_1) p_1^\varphi \Psi\rangle + \langle p_1^\varphi \Psi, w(x_1) q_1^\varphi \Psi\rangle + \langle q_1^\varphi \Psi, w(x_1) p_1^\varphi \Psi\rangle \\ &\quad + \langle q_1^\varphi \Psi, w(x_1) q_1^\varphi \Psi\rangle - \langle \varphi, w\varphi\rangle\big| \\ &\leq \langle \varphi, w\varphi\rangle \left(1 - \|p_1^\varphi \Psi\|^2\right) + \|w\|_\infty \|q_1^\varphi \Psi\|^2 + 2|\langle q_1^\varphi \Psi, w(x_1) p_1^\varphi \Psi\rangle| \\ &\leq 2\|w\|_\infty \|q_1^\varphi \Psi\|^2 + 2\|(\widehat{n}^\varphi)^{-1/2} q_1^\varphi \Psi\| \, \|(\widehat{n}^\varphi)^{1/2} w(x_1) p_1^\varphi \Psi\| .\end{aligned}$$

Using that $\sqrt{k+1} < \sqrt{k}+1$ (thus $n(k+1) < n(k) + N^{-1/2}$) and part (d)

$$\begin{aligned}
\|(\widehat{n}^\varphi)^{1/2} w(x_1) p_1^\varphi \Psi\|^2 &= \langle \Psi, p_1^\varphi w(x_1) \widehat{n}^\varphi q_1^\varphi w(x_1) p_1^\varphi \Psi\rangle + \langle \Psi, p_1^\varphi w(x_1) \widehat{n}^\varphi p_1^\varphi w(x_1) p_1^\varphi \Psi\rangle \\
&= \langle (\widehat{n}^\varphi)^{1/2}\Psi, p_1^\varphi w(x_1) q_1^\varphi w(x_1) p_1^\varphi (\widehat{n}^\varphi)^{1/2}\Psi\rangle \\
&\quad + \langle (\widehat{n}^\varphi_{-1})^{1/2}\Psi, p_1^\varphi w(x_1) p_1^\varphi w(x_1) p_1^\varphi (\widehat{n}^\varphi_{-1})^{1/2}\Psi\rangle \\
&\leq \|w(x_1)\|_\infty^2 \left(2\|(\widehat{n}^\varphi)^{1/2}\Psi\|^2 + N^{-1/2}\right)
\end{aligned}$$

thus part (c) of the Lemma yields

$$|\langle \Psi, w(x_1)\Psi\rangle - \langle \varphi, w\varphi\rangle| \leq 4\|w\|_\infty \left(\|\widehat{n}^\varphi \Psi\|^2 + N^{-1/4} + \|(\widehat{n}^\varphi)^{1/2}\Psi\|^2\right)$$

With the operator inequality $(\widehat{n}^\varphi)^\lambda < (\widehat{n}^\varphi)^\gamma$ for any $\lambda < \gamma$ we get (e).

□

2.1 Convergence of the Reduced Density Matrix

Lemma 2.4 *Let $j > 0$, $\varphi \in L^2$ and let $\Psi \in L^2(\mathbb{R}^{3N} \to \mathbb{C})$ be symmetric, let $\mu(\Psi)$ be the reduced one particle density matrix of Ψ. Then*

(a)

$$\lim_{N\to\infty} \|\widehat{n}^\varphi \Psi\| = 0 \Leftrightarrow \lim_{N\to\infty} \left\langle \Psi, (\widehat{n}^\varphi)^j\, \Psi \right\rangle = 0\ .$$

(b)

$$\lim_{N\to\infty} \left\langle \Psi, (\widehat{n}^\varphi)^j\, \Psi \right\rangle = 0 \Rightarrow \lim_{N\to\infty} \mu(\Psi) = |\varphi\rangle\langle\varphi|$$

in weak-$\star$ sense.

Proof: We shall show that

$$\lim_{N\to\infty} \langle \Psi, (\widehat{n}^\varphi)^l\, \Psi\rangle = 0 \Rightarrow \lim_{N\to\infty} \left\langle \Psi, (\widehat{n}^\varphi)^j\, \Psi \right\rangle = 0$$

for any $j, l > 0$, which is equivalent to (a).

Let $\lim_{N\to\infty}\langle \Psi, (\widehat{n}^\varphi)^j \Psi\rangle = 0$ for some $j > 0$. It follows, that there exists a function $\delta(N)$ with $\lim_{N\to\infty} \delta(N) = 0$ such that

$$\sum_{k=0}^{N} \left(\frac{k}{N}\right)^j \|P_k \Psi\| < \delta(N)\ .$$

Let $k(N)$ be the smallest integer such that $\left(\frac{k(N)}{N}\right)^j < \sqrt{\delta(N)}$. It follows that $\left(\frac{k(N)+1}{N}\right)^j \geq \sqrt{\delta(N)}$ and thus $\sum_{k(N)+1}^{N} \|P_k \Psi\| < \sqrt{\delta(N)}$. Hence

$$\begin{aligned}
\sum_{k=0}^{N} \left(\frac{k}{N}\right)^l \|P_k \Psi\| &= \sum_{k=0}^{k(N)} \left(\frac{k}{N}\right)^l \|P_k \Psi\| + \sum_{k(N)+1}^{N} \|P_k \Psi\| \\
&\leq \left(\frac{k(N)}{N}\right)^l + \sqrt{\delta(N)} \leq \left(\sqrt{\delta(N)}\right)^{l/j} + \sqrt{\delta(N)}\ .
\end{aligned}$$

Thus $\lim_{N\to\infty} \left\langle \Psi, (\widehat{n}^{\varphi})^j \, \Psi \right\rangle = 0$ and (a) follows.

With (a) we can choose without loss of generality $j = 2$ to prove (b). So let

$$\lim_{N\to\infty} \left\langle \Psi, (\widehat{n}^{\varphi})^2 \Psi \right\rangle = 0 \, .$$

With Lemma 2.3 (c) we have using symmetry of Ψ_t that $\lim_{N\to\infty} \|q_1^{\varphi}\Psi\| = 0$ and $\lim_{N\to\infty} \|p_1^{\varphi}\Psi\| = 1$. Note, that

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

The first summand equals $\|p_1^{\varphi}\Psi\|^2 \; |\varphi\rangle\langle\varphi|$, the other summands have operator norm $\|q_1^{\varphi}\Psi\| \; \|p_1^{\varphi}\Psi\|$ and $\|q_1^{\varphi}\Psi\|^2$ respectively and the Lemma follows.

□

Remark 2.5 *Similarly one can proof that* $\lim_{N\to\infty} \langle \Psi, (\widehat{n}^{\varphi})^{\gamma} \Psi \rangle = 0$ *for* $\gamma \in \mathbb{R}^+$ *implies convergence of the reduced* k*-particle density matrix for any fixed* $k < \infty$*.*

3 Derivation of the Hartree equation

Let us now consider the different cases for β. To motivate the technique we shall use below, we first take a short look at $\beta = 0$. In this case we have that the mean field is of the form $v \star |\varphi_t|^2$ and (3) becomes the Hartree equation.

Let φ_t be a solution of the Hartree equation, let $T < \infty$ be such that $\|\varphi_t\|_\infty < \infty$ for all $t < T$.

Defining

$$\alpha_t := \|\widehat{n}^{\varphi_t}\Psi_t\| = \langle \Psi_t, (\widehat{n}^{\varphi_t})^2 \Psi_t \rangle \tag{8}$$

and assuming that $\alpha_0 \to 0$ as $N \to \infty$ we wish to show that $\alpha_t \to 0$ uniform in $t < T$.

Note, that α_t is $1/N$ times the expectation of particles which are not in the state φ_t, i.e. $1 - \alpha_t = \langle \Psi_t, \left(1 - (\widehat{n}^{\varphi_t})^2\right) \Psi_t \rangle$ is $1/N$ times the expectation of particles which are in the state φ_t.

By (8)

$$\alpha_t' = \frac{d}{dt}\alpha_t := -i\langle \Psi_t, [H - H^H, (\widehat{n}^{\varphi_t})^2] \Psi_t \rangle$$

where

$$H^H := \sum_{j=1}^{N} -\Delta_j + A_t(x_j) + (v \star |\varphi_t|^2)(x_j) \ .$$

Using symmetry of Ψ_t and Definition 2.1 we have

$$\begin{aligned}
\alpha_t' &= -iN^{-1}\sum_{j=1}^{N}\langle\Psi_t,[\sum_{k\neq l} v_\beta^N(x_k-x_l) - \sum_{l=1}^{N} v\star|\varphi_t|^2(x_l), q_j^{\varphi_t}]\Psi_t\rangle \\
&= -i\langle\Psi_t,[\sum_{k\neq 1} v_\beta^N(x_k-x_1) - v\star|\varphi_t|^2(x_1), q_1^{\varphi_t}]\Psi_t\rangle \\
&= -i\langle\Psi_t,\big((N-1)v_\beta^N(x_2-x_1) - v\star|\varphi_t|^2(x_1)\big)q_1^{\varphi_t}\Psi_t\rangle \\
&\quad +i\langle\Psi_t,q_1^{\varphi_t}\big(v_\beta^N(x_2-x_1) - v\star|\varphi_t|^2(x_1)\big)\Psi_t\rangle \\
&= -i\big(\langle\Psi_t,q_1^{\varphi_t}\big((N-1)v_\beta^N(x_2-x_1) - v\star|\varphi_t|^2(x_1)\big)q_1^{\varphi_t}\Psi_t\rangle \\
&\quad -i\langle\Psi_t,p_1^{\varphi_t}\big((N-1)v_\beta^N(x_2-x_1) - v\star|\varphi_t|^2(x_1)\big)q_1^{\varphi_t}\Psi_t\rangle \\
&\quad +i\langle\Psi_t,q_1^{\varphi_t}\big((N-1)v_\beta^N(x_2-x_1) - v\star|\varphi_t|^2(x_1)\big)q_1^{\varphi_t}\Psi_t\rangle \\
&\quad +i\langle\Psi_t,q_1^{\varphi_t}\big((N-1)v_\beta^N(x_2-x_1) - v\star|\varphi_t|^2(x_1)\big)p_1^{\varphi_t}\Psi_t\rangle\big)
\end{aligned}$$

Using selfadjointness of the multiplication operators the first and third summand cancel out and we get

$$|\alpha_t'| \leq 2|\langle\Psi_t,p_1^{\varphi_t}\big((N-1)v_\beta^N(x_2-x_1) - v\star|\varphi_t|^2(x_1)\big)q_1^{\varphi_t}\Psi_t\rangle|$$

Using $\langle\Psi,p_2^{\varphi_t}v_\beta^N(x_1-x_2)p_2^{\varphi_t}\Psi\rangle = \langle\Psi,(v\star|\varphi_t|^2)(x_1)p_2^{\varphi_t}\Psi\rangle$ and Lemma 2.3 (d)

$$\begin{aligned}
|\alpha_t'| &\leq 2|\langle\Psi_t,p_1^{\varphi_t}p_2^{\varphi_t}\big((N-1)v_\beta^N(x_2-x_1) - v\star|\varphi_t|^2(x_1)\big)q_1^{\varphi_t}q_2^{\varphi_t}\Psi_t\rangle| \\
&\quad +2|\langle\Psi_t,p_1^{\varphi_t}q_2^{\varphi_t}\big((N-1)v_\beta^N(x_2-x_1) - v\star|\varphi_t|^2(x_1)\big)q_1^{\varphi_t}p_2^{\varphi_t}\Psi_t\rangle| \\
&\quad +2|\langle\Psi_t,p_1^{\varphi_t}q_2^{\varphi_t}\big((N-1)v_\beta^N(x_2-x_1) - v\star|\varphi_t|^2(x_1)\big)q_1^{\varphi_t}q_2^{\varphi_t}\Psi_t\rangle| \\
&\leq 2|\langle\Psi_t,\widehat{n}_2^{\varphi_t}p_1^{\varphi_t}p_2^{\varphi_t}\big((N-1)v_\beta^N(x_2-x_1) - v\star|\varphi_t|^2(x_1)\big)(\widehat{n}^{\varphi_t})^{-1}q_1^{\varphi_t}q_2^{\varphi_t}\Psi_t\rangle| \\
&\quad +2\left(\|p_1^{\varphi_t}q_2^{\varphi_t}\Psi_t\|^2 + \|p_1^{\varphi_t}q_2^{\varphi_t}\Psi_t\|\ \|q_1^{\varphi_t}q_2^{\varphi_t}\Psi_t\|\right)\left(\left\|(N-1)v_\beta^N\right\|_\infty + \left\|v\star|\varphi_t|^2\right\|_\infty\right) \ .
\end{aligned}$$

Remember that in the case $\beta=0$ the scaling is such that $v_\beta^N = N^{-1}v$, thus $\|v_\beta^N\|_1 = N^{-1}\|v\|_1$ and $\|v_\beta^N\|_\infty = N^{-1}\|v\|_\infty$. Note also that $\frac{\sqrt{j+2}}{\sqrt{N}} < \frac{\sqrt{j}}{\sqrt{N}} + \frac{2}{\sqrt{N}}$ and thus $\widehat{N}_2^{\varphi_t} \leq \widehat{n}^{\varphi_t} + \frac{2}{\sqrt{n}}$. It follows that

$$\begin{aligned}
|\alpha_t'| &\leq C\left\|\left(\widehat{n}_t^{\varphi} + \frac{2}{\sqrt{N}}\right)\Psi_t\right\|\ \|(\widehat{n}^{\varphi_t})^{-1}q_1^{\varphi_t}q_2^{\varphi_t}\Psi_t\| \\
&\qquad +2C\left(\|p_1^{\varphi_t}q_2^{\varphi_t}\Psi_t\|^2 + \|p_1^{\varphi_t}q_2^{\varphi_t}\Psi_t\|\ \|q_1^{\varphi_t}q_2^{\varphi_t}\Psi_t\|\right) \ .
\end{aligned}$$

Using Lemma 2.3 (c) it follows in view of (8) that one can find a $C<\infty$ such that

$$|\alpha_t'| \leq C\alpha + CN^{-1/2} \ ,$$

thus by Gronwalls Lemma $\alpha_t \to 0$ for $N\to\infty$ uniform in $t<T$ (under the assumptions above, in particular $\alpha_0 \to 0$ for $N\to\infty$).

4 Derivation of the Gross-Pitaevskii equation

Let us now consider the case $0 < \beta \leq 1$. Then (3) becomes the Gross Pitaevskii equation

$$i\frac{d}{dt}\varphi_t^{GP} = (-\Delta + A_t)\,\varphi_t^{GP} + 2a|\varphi_t^{GP}|^2\varphi_t^{GP} := h^{GP}\varphi_t^{GP} \;. \tag{9}$$

The respective Gross Pitaevskii energy is given by

$$\begin{aligned} E_t^{GP} &= E_t^{kin} + E_t^{pot} := \langle \nabla\varphi_t^{GP}, \nabla\varphi_t^{GP}\rangle + \langle \varphi_t^{GP}, (A_t + a|\varphi_t^{GP}|^2)\varphi_t^{GP}\rangle \\ &= \langle \varphi_t^{GP}, (h^{GP} - a|\varphi_t^{GP}|^2)\varphi_t^{GP}\rangle \;. \end{aligned} \tag{10}$$

To control $\langle \Psi_t, \widehat{n}^{\varphi_t^{GP}}\Psi_t\rangle$, the solutions φ_t^{GP} of the Gross Pitaevskii equation we shall consider have to satisfy some additional conditions. If we have in addition sufficiently strong decay conditions on φ_t^{GP} in t we can even get control on the respective α_t uniform in $t < \infty$. Therefore we shall define next the sets $\mathcal{G}$ and $\mathcal{G}_{dec}$ of solutions of (9) which satisfy these conditions

Definition 4.1

$$\mathcal{G} := \{\varphi_t^{GP} : i\frac{d}{dt}\varphi_t^{GP} = h^{GP}\varphi_t^{GP};\ \|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty + \|\Delta\varphi_t^{GP}\|_\infty < \infty\ \forall\, t \geq 0\}$$

and

$$\mathcal{G}_{dec} := \{\varphi_t^{GP} \in \mathcal{G} : \int_0^\infty \|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty dt < \infty\}$$

Furthermore we shall — depending on β — need some conditions on the interaction v_β^N. These conditions shall include the potentials we used in the introduction, i.e. potentials which scale like $v_\beta^N(x) = N^{-1+3\beta}v(N^\beta x)$ for a compactly supported, spherically symmetric, positive potential $v \in L^1 \cap L^\infty$.

Definition 4.2 *For any $0 < \beta \leq 1$ let*

$$\mathcal{W}_\beta := \{v_\beta^N \textit{ pos. and spher. symm. } v_\beta^N(x) = 0\ \forall\, x > RN^{-\beta} \textit{ for some } R < \infty\} \;.$$

For any $0 < \beta < 1$ let

$$\begin{aligned} \mathcal{V}_\beta := \{v_\beta^N \in \mathcal{W}_\beta : \quad & \lim_{N\to\infty} N^{1-3\beta}\|v_\beta^N\|_\infty < \infty; \\ & \lim_{N\to\infty} N^{1+\delta}(\|v_\beta^N\|_1 - a/N) < \infty \textit{ for some } \delta > 0\} \end{aligned}$$

and let

$$\mathcal{V}_1 := \{v_\beta^N \in \mathcal{W}_1 : \lim_{N\to\infty} N^{1+\delta}(scat(v_\beta^N) - a/N) < \infty \textit{ for some } \delta > 0\} \;,$$

where $scat(v)$ is the scattering length of the potential v.

With these definitions we arrive at the main Theorem:

Theorem 4.3 *Let $0 < \beta \leq 1$, let $v_\beta^N \in \mathcal{V}_\beta$ and let $\varphi_t^{GP} \in \mathcal{G}$. Let $T < \infty$ ($T \leq \infty$ if $\varphi_t^{GP} \in \mathcal{G}_{dec}$). Let A_t be such that $\int_0^T \|A_t'\| dt < \infty$. Let Ψ_0 be symmetric with $\|\Psi_0\| = 1$,*

$$\lim_{N\to\infty} N^\delta \left\langle \Psi_0, \left(\widehat{n}^{\varphi_t^{GP}}\right)^2 \Psi_0 \right\rangle = 0 \tag{11}$$

and

$$\lim_{N\to\infty} N^\delta (N^{-1}\langle \Psi_0, H\Psi_0\rangle - E_t^{GP}) = 0 \tag{12}$$

for some $\delta > 0$. Then

$$\lim_{N\to\infty} \left\langle \Psi_t, \left(\widehat{n}^{\varphi_t^{GP}}\right)^2 \Psi_t \right\rangle = 0 \tag{13}$$

uniform in $0 < t < T$.

Remark 4.4 *(a) Lemma 2.4 implies convergence of the reduced one-particle density matrix.*

(b) For $\beta = 1$ the conditions on v_β^N include the hard sphere case (and potentials which scale like $v_\beta^N = N^\gamma v(Nx)$ for any $\gamma > 2$) with compactly supported v with support-radius a: Such potentials satisfy all conditions one needs to be in $\mathcal{W}_1$ and the respective scattering length equals a/N (converges against a/N) as $N \to \infty$.

(c) It has been proven for a large class of external potentials that the N-particle ground state wave function Ψ satisfies the conditions (11) and (12) [5, 6, 7]. So the Theorem fits well for describing the physics of a trapped, cooled Bose gas when the trap is removed.

(d) Condition (12) can be understood as smoothness condition on Ψ_0. For the case $0 < \beta < 1$ this is clear on a heuristic level: If all particles of Ψ_0 are more or less equal to φ_t^{GP} and if Ψ_0 is smooth enough, then the energy of Ψ_0 is of course close to NE_t^{GP}.

For $\beta = 1$ note, that L^2 density arguments can be used, i.e. if (13) holds for some Ψ_0, then it also holds for a sequence Ψ_0^N which converges in L^2 against Ψ_0. Thus we can equip Ψ_0 with a microscopic structure which does not change the L^2 norm significantly in such a way, that the energy gets close to NE_t^{GP}.

With the technique we shall present in this paper this can be done rigorously.

4.1 Proof of the Theorem

Notation 4.5 *In the following all projectors shall be with respect to φ_t^{GP}. We shall omit the upper index φ_t^{GP} on p_j, q_j, P_j, $P_{j,k}$ and $\widehat{\cdot}$.*

Note that due to Lemma 2.4 (a) we have some flexibility in choosing which term we wish to control: To prove the Theorem we can choose to control $\langle\Psi_t, (\widehat{n})^\gamma \Psi_t\rangle$ for arbitrary $\gamma > 0$. We shall use $\gamma = 1$ since we shall estimate the kinetic energy (see Lemma 5.4 below) in terms of $\langle\Psi_t, \widehat{n}\ \Psi_t\rangle$.

Definition 4.6 *Using the notation*

$$h_{j,k} := (N-1)v_\beta^N(x_j - x_k) - \frac{a}{2}|\varphi_t^{GP}|^2(x_j) - \frac{a}{2}|\varphi_t^{GP}|^2(x_k)$$

we define the functional $\alpha : L^2(\mathbb{R}^{3N} \to \mathbb{C}) \to \mathbb{R}^+$ *by*

$$\alpha(\Psi) := \langle\Psi, \widehat{n}\Psi\rangle = \|(\widehat{n})^{1/2}\Psi\|$$

and the functionals $\alpha'_{1,2} : L^2(\mathbb{R}^{3N} \to \mathbb{C}) \to \mathbb{R}^+$ *by*

$$\alpha'_1(\Psi) = N\Im\left(\langle\Psi, h_{1,2}(\widehat{n} - \widehat{n}_2)p_1p_2\Psi\rangle\right) \tag{14}$$

$$\alpha'_2(\Psi) = N\Im\left(\langle\Psi, h_{1,2}(\widehat{n} - \widehat{n}_1)p_1q_2\Psi\rangle\right) \ . \tag{15}$$

Lemma 4.7 *For any solution of the Schrödinger equation* Ψ_t *we have*

$$\frac{d}{dt}\alpha(\Psi_t) = 2\alpha'_1(\Psi_t) + 4\alpha'_2(\Psi_t) \ .$$

Proof: We have for $0 < \beta \leq 1$ for the time derivative

$$\begin{aligned} \frac{d}{dt}\alpha(\Psi) &= \frac{d}{dt}\langle\Psi, \widehat{n}\ \Psi\rangle \\ &= -i\langle H^\beta\Psi, \widehat{n}\ \Psi\rangle + i\langle\Psi, \widehat{n}\ H^\beta\Psi\rangle + i\langle\Psi, [H_t^{GP}, \widehat{n}\ ]\Psi\rangle \\ &= -i\langle\Psi, [H^\beta - H_t^{GP}, \widehat{n}\ ]\Psi\rangle \ . \end{aligned}$$

Using symmetry of Ψ it follows that

$$\begin{aligned} \frac{d}{dt}\alpha(\Psi) &= -i(N-1)^{-1}\sum_{j\neq k}\langle\Psi, [h_{j,k}, \widehat{n}\ ]\Psi\rangle \\ &= -iN\langle\Psi, h_{1,2}\widehat{n}\ \Psi\rangle - \langle\Psi, \widehat{n}\ h_{1,2}\Psi\rangle = 2N\Im\left(\langle\Psi, h_{1,2}\widehat{n}\ \Psi\rangle\right) \ . \end{aligned} \tag{16}$$

Note that we can write for any $m : \{1, \ldots, N\} \to \mathbb{R}^+$

$$\begin{aligned}
\widehat{m} &= \sum_{k=0}^{N} m(k) P_k \qquad (17)\\
&= \sum_{k=0}^{N-2} \big(m(k) p_1 p_2 P_{N-2,k} + m(k) p_1 q_2 P_{N-2,k-1} \\
&\quad + m(k) q_1 p_2 P_{N-2,k-1} + m(k)(1 - p_1 q_2 - q_1 p_2 - p_1 p_2) P_{N-2,k-2} \big) \\
&= \sum_{k=0}^{N} \big(m(k) p_1 p_2 P_{N-2,k} + m(k) p_1 q_2 P_{N-2,k-1} \\
&\quad + m(k) q_1 p_2 P_{N-2,k-1} + m(k) P_{N-2,k-2} \big) \\
&\quad - \sum_{k=0}^{N} m(k+1) p_1 q_2 P_{N-2,k-1} - m(k+1) q_1 p_2 P_{N-2,k-1} \\
&\quad - m(k+2) p_1 p_2 P_{N-2,k}) \\
&= (\widehat{m} - \widehat{m}_2) p_1 p_2 + (\widehat{m} - \widehat{m}_1) p_1 q_2 + (\widehat{m} - \widehat{m}_1) q_1 p_2 + \sum_{k=0}^{N} m(k) P_{N-2,k-2}
\end{aligned}$$

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

$$\frac{d}{dt} \alpha(\Psi) = \Im \left(\langle \Psi, h_{1,2} \left(N(\widehat{n} - \widehat{n}_2) p_1 p_2 + 2(\widehat{n} - \widehat{n}_1) p_1 q_2 \right) \Psi \rangle \right) \ .$$

□

5 The Gross Pitaevskii equation for $0 < \beta < 1/3$

In this section we shall control $\alpha_{1,\Psi}$ and $\alpha_{2,\Psi}$ under additional conditions on β, namely $\beta < 1/3$ for $\alpha_{1,\Psi}$ and $\beta < 1$ for $\alpha_{2,\Psi}$.

Lemma 5.1 *We have under the conditions of Theorem 4.3 that there exists a $C < \infty$ and a $\xi > 0$ such that for any $\Psi \in L^2(\mathbb{R}^{3N} \to \mathbb{C})$ with $\nabla_1 \Psi \in L^2(\mathbb{R}^{3N} \to \mathbb{C})$ that*

(a) for $0 < \beta < 1/3$

$$|\alpha_1'(\Psi)| \leq C(\|\varphi_t^{GP}\|_\infty + \|\nabla \varphi_t^{GP}\|_\infty)(\alpha(\Psi) + N^{-\xi})$$

(b) for $0 < \beta < 1$

$$|\alpha_2'(\Psi)| \leq C(\|\varphi_t^{GP}\|_\infty + \|\nabla \varphi_t^{GP}\|_\infty)(\alpha(\Psi) + \|\nabla_1 q_1 \Psi\| + N^{-\xi})$$

Proof: Using (14) and $1 = p_1p_2 + p_1q_2 + q_1p_2 + q_1q_2$

$$\begin{aligned}\alpha_1'(\Psi) &= \Im\left(\langle\Psi, p_1p_2h_{1,2}N(\widehat{n}-\widehat{n}_2)p_1p_2\Psi\rangle\right) + \Im\left(\langle\Psi, p_1q_2h_{1,2}N(\widehat{n}-\widehat{n}_2)p_1p_2\Psi\rangle\right)\\ &\quad+\Im\left(\langle\Psi, q_1p_2h_{1,2}N(\widehat{n}-\widehat{n}_2)p_1p_2\Psi\rangle\right) + \Im\left(\langle\Psi, q_1q_2h_{1,2}N(\widehat{n}-\widehat{n}_2)p_1p_2\Psi\rangle\right)\\ \alpha_2'(\Psi) &= \Im\left(\langle\Psi, p_1p_2h_{1,2}N(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\rangle\right) + \Im\left(\langle\Psi, p_1q_2h_{1,2}N(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\rangle\right)\\ &\quad+\Im\left(\langle\Psi, q_1p_2h_{1,2}N(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\rangle\right) + \Im\left(\langle\Psi, q_1q_2h_{1,2}N(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\rangle\right)\ .\end{aligned}$$

Using that $\Im(\langle\Psi, A\Psi\rangle) = -\Im(\langle\Psi, A^t\Psi\rangle)$ for any operator A and that Ψ is symmetric (note that $p_1q_2h_{1,2}q_1p_2$ is invariant under adjunction plus exchange of the variable x_1 and x_2) and Lemma 2.3 (dc) we get

$$\begin{aligned}\alpha_1'(\Psi) &= 2\Im\left(\langle\Psi, p_1q_2h_{1,2}N(\widehat{n}-\widehat{n}_2)p_1p_2\Psi\rangle\right) + \Im\left(\langle\Psi, q_1q_2h_{1,2}N(\widehat{n}-\widehat{n}_2)p_1p_2\Psi\rangle\right)\\ \alpha_2'(\Psi) &= \Im\left(\langle\Psi, N(\widehat{n}_1-\widehat{n}_2)p_1p_2h_{1,2}p_1q_2\Psi\rangle\right) + \Im\left(\langle\Psi, q_1q_2h_{1,2}N(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\rangle\right)\end{aligned}$$

Note that

$$\begin{aligned}\sqrt{k/N} - \sqrt{(k-2)/N} &= (k/N - (k-2)/N)\,/\left(\sqrt{k/N} + \sqrt{(k-2)/N}\right)\\ &\le (2/N)/(\sqrt{k/N}) = 2(Nk)^{-1/2}\ ,\end{aligned}$$

so we have that $0 \le (\widehat{n}-\widehat{n}_1), (\widehat{n}_1-\widehat{n}_2) \le (\widehat{n}-\widehat{n}_2) \le 2(N\widehat{n})^{-1}$ and Lemma 5.1 follows from

Lemma 5.2 *Let $m : \{1,\dots,N\} \to \mathbb{R}^+$ with $m \le n^{-1}$, $0 < \beta < 1$. Then we have under the conditions of the Theorem that there exists a $C < \infty$ and a $\xi > 0$ such that*

(a) for any $0 < \beta < 1$

$$\begin{aligned}&|\langle\Psi_t, p_1p_2h_{1,2}\widehat{m}q_1p_2\Psi_t\rangle| \le C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)N^{-\xi}\\ &|\langle\Psi_t, p_1q_2\widehat{m}^{1/2}h_{1,2}\widehat{m}^{1/2}q_1q_2\Psi_t\rangle|\\ &\qquad\le C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)(\alpha(\Psi) + N^{-\gamma} + \|\nabla_1q_1\Psi\|^2)\end{aligned}$$

(b) for any $0 < \beta < 1/3$

$$|\langle\Psi_t, p_1p_2\widehat{m}^{1/2}h_{1,2}\widehat{m}^{1/2}q_1q_2\Psi_t\rangle| \le C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)(\alpha(\Psi_t) + N^{-\xi})$$

The proof of Lemma 5.2 shall be given in the Appendix for later reference in a more general form.

□

5.1 Control of the kinetic energy for $\beta < 1$

To finish the control of $\alpha(\Psi_t)$ we shall provide a sufficient estimate on the kinetic energy of Ψ_t, in particular $\|\nabla_1q_1\Psi_t\|$. This estimate shall be given in terms of $\alpha(\Psi_t)$, thus finally our estimate on $\alpha'(\Psi_t)$ shall depend on α_Ψ making $\alpha(\Psi_t)$ controllable by a Gronwall argument. For that we need

Lemma 5.3 *Let $m : \{1, \ldots, N\} \to \mathbb{R}^+$ with $m \leq n^{-1}$, $0 < \beta < 1$. Then we have under the conditions of the Theorem that there exists a $C < \infty$ and a $\xi > 0$ such that for any $0 < \beta < 1$*

$$|\langle \Psi, p_1 p_2 \left((N-1) v_\beta^N(x_1, x_2) - a|\varphi_t^{GP}|^2(x_1)\right) p_1 p_2 \Psi\rangle| \leq C(\|\varphi_t^{GP}\|_\infty + \|\nabla \varphi_t^{GP}\|_\infty) N^{-\xi}$$

and

$$|\langle \Psi, p_1 p_2 v_\beta^N(x_1, x_2) q_1 q_2 \Psi\rangle| \leq C N^{-1}(\|\varphi_t^{GP}\|_\infty + \|\nabla \varphi_t^{GP}\|_\infty)(\alpha(\Psi) + N^{-\xi}) \; .$$

The proof of which shall be given together with the proof of Lemma 5.2 in the Appendix.

Lemma 5.4 *Let $0 < \beta < 1$. Then we have under the conditions of Theorem 4.3 that there exists a $\xi > 0$ such that uniform in $0 < t < T$*

$$\|\nabla_1 q_1 \Psi_t\|^2 \leq C \left(\sup_{0 \leq s \leq t} \{\alpha(\Psi_s)\} + N^{-\xi} \right)$$

Proof: Using symmetry of Ψ_t

$$N^{-1}\langle \Psi_t, H\Psi_t\rangle = -\|\nabla_1 \Psi_t\|^2 + (N-1)\langle \Psi_t, v_\beta^N(x_1 - x_2)\Psi_t\rangle + \langle \Psi_t, A_t(x_1)\Psi_t\rangle \; ,$$

Thus

$$\begin{aligned} &\|\nabla \varphi_t^{GP}\|^2 - \|\nabla_1 \Psi_t\|^2 = N^{-1}\langle \Psi_t, H\Psi_t\rangle - E_t^{GP} - \langle \Psi_t, \left(A_t(x_1) + a|\varphi_t^{GP}|^2(x_1)\right)\Psi_t\rangle \\ &+\langle \varphi_t^{GP}, \left(A_t + a|\varphi_t^{GP}|^2\right)\varphi_t^{GP}\rangle + \left\langle \Psi_t, \left((N-1)v_\beta^N(x_1 - x_2) - a|\varphi_t^{GP}|^2(x_1)\right)\Psi_t\right\rangle \; . \end{aligned}$$

Using symmetry of Ψ_t

$$\begin{aligned} & \frac{d}{dt}\left(N^{-1}\langle \Psi_t, H\Psi_t\rangle - E_t^{GP}\right) = \langle \Psi_t, A_t'(x_1)\Psi_t\rangle - \langle \varphi_t^{GP}, a\left(\frac{d}{dt}|\varphi_t^{GP}|^2\right)\varphi_t^{GP}\rangle \\ & -\langle \varphi_t^{GP}, A_t'\varphi_t^{GP}\rangle - \langle \varphi_t^{GP}, [(h^{GP} - a|\varphi_t^{GP}|^2), h^{GP}]\varphi_t^{GP}\rangle \\ = \; & \langle \Psi_t, A_t'(x_1)\Psi_t\rangle - \langle \varphi_t^{GP}, A_t'\varphi_t^{GP}\rangle + \langle \varphi_t^{GP}, [a|\varphi_t^{GP}|^2, h^{GP}]\varphi_t^{GP}\rangle \\ & -\langle \varphi_t^{GP}, [a|\varphi_t^{GP}|^2, h^{GP}]\varphi_t^{GP}\rangle \\ \leq \; & 4\|A_t'\|_\infty \left(N^{-1/4} + \alpha(\Psi_t)\right) \; , \end{aligned}$$

where we used Lemma 2.3 (e) in the last step. It follows using condition (12) that for N sufficiently small (i.e. such that $N^\delta\left(N^{-1}\langle \Psi_0, H\Psi_0\rangle - E_0^{GP}\right) < 1$)

$$\begin{aligned} \left(N^{-1}\langle \Psi_t, H\Psi_t\rangle - E_t^{GP}\right) \; &< \; N^{-\delta} + \int_0^t \|A_s'\|_\infty \left(\left(\frac{2}{N}\right)^{1/4} + \alpha(\Psi_s)\right) ds \\ &\leq \; C(N^{-\delta} + N^{-1/4} + \sup_{0 \leq s \leq t}\{\alpha(\Psi_s)\}) \end{aligned}$$

uniform in $t < T$. Note that due to Lemma 2.3 (e)

$$\begin{aligned} & \langle \Psi_t, \left(A_t(x_1) + a|\varphi_t^{GP}|^2(x_1)\right) \Psi_t\rangle - \langle \varphi_t^{GP}, \left(A_t + a|\varphi_t^{GP}|^2\right) \varphi_t^{GP}\rangle \\ \leq \; & 4(\|A_t\|_\infty + a\|\varphi_t^{GP}\|_\infty^2) \left(N^{-1/4} + \alpha(\Psi_t)\right) , \end{aligned}$$

thus

$$\begin{aligned} \left|\|\nabla_1 \Psi_t\|^2 - \|\nabla \varphi_t^{GP}\|^2\right| \;\leq\; & C(N^{-\delta} + N^{-1/4} + \sup_{0\leq s\leq t}\{\alpha(\Psi_s)\}) \\ & + \left|\left\langle \Psi_t, \left((N-1)v_\beta^N(x_1 - x_2) - a|\varphi_t^{GP}|^2(x_1)\right) \Psi_t\right\rangle\right| . \end{aligned} \tag{18}$$

We get using symmetry of Ψ_t and self adjointness of the multiplication operators for the last summand in (18)

$$\begin{aligned} & \left\langle \Psi_t, \left((N-1)v_\beta^N(x_1 - x_2) - a|\varphi_t^{GP}|^2(x_2)\right) \Psi_t\right\rangle \\ = \; & \left\langle p_1p_2\Psi_t, \left((N-1)v_\beta^N(x_1 - x_2) - a|\varphi_t^{GP}|^2(x_2)\right) p_1p_2\Psi_t\right\rangle \\ & + 2\Re \left\langle p_1p_2\Psi_t, (N-1)v_\beta^N(x_1 - x_2) - a|\varphi_t^{GP}|^2(1 - p_1p_2)\Psi_t\right\rangle \\ & + (N-1) \left\langle (1 - p_1p_2)\Psi_t, v_\beta^N(x_1 - x_2)(1 - p_1p_2)\Psi_t\right\rangle \qquad (19) \\ & - a \left\langle (1 - p_1p_2)\Psi_t, |\varphi_t^{GP}|^2(1 - p_1p_2)\Psi_t\right\rangle . \end{aligned}$$

Using symmetry of Ψ_t, the absolute value of the second term is bounded by

$$\begin{aligned} & 4(N-1) \left|\left\langle p_1p_2\Psi_t, (N-1)v_\beta^N(x_1 - x_2) - a|\varphi_t^{GP}|^2 p_1q_2\Psi_t\right\rangle\right| \\ + \; & 2(N-1) \left|\left\langle p_1p_2\Psi_t, v_\beta^N(x_1 - x_2)q_1q_2\Psi_t\right\rangle\right| \end{aligned}$$

Using Lemma 5.2 in its more general form as given in the Appendix and using positivity of v_β^N (implying positivity of line (19)) we get that

$$\begin{aligned} & \left\langle \Psi_t, \left(\sum_{j\neq 1} v_\beta^N(x_j - x_1) - a|\varphi_t^{GP}|^2\right) \Psi_t\right\rangle \\ \geq \; & -C(\alpha(\Psi_t) + N^{-\xi}) - a\|\varphi_t^{GP}\|_\infty^2 \, \|(1 - p_1p_2)\Psi_t\|^2 . \end{aligned}$$

Writing $1 - p_1p_2 = p_1q_2 + q_1p_2 + q_1q_2$ Lemma 2.3 yields

$$\left\langle \Psi_t, \left(\sum_{j\neq 1} v_\beta^N(x_j - x_1) - a|\varphi_t^{GP}|^2\right) \Psi_t\right\rangle \geq -C(\alpha(\Psi_t) + N^{-\xi} + N^{-\delta} + N^{\beta-1}) , \tag{20}$$

so with (18)

$$\left|\|\nabla_1 \Psi_t\|^2 - \|\nabla \varphi_t^{GP}\|^2\right| \;\leq\; C(N^{-\delta} + N^{-1/4} + \sup_{0\leq s\leq t}\{\alpha(\Psi_s)\} + N^{-\beta} + N^{\beta-1}) .$$

Note also that $\|\nabla \Psi_t\|^2 = \|\nabla p_1\Psi_t\|^2 + \|\nabla q_1\Psi_t\|^2$ and

$$\begin{aligned} \|\nabla p_1\Psi_t\|^2 - \|\nabla p_1\Psi_t\|^2 \;=\; & \|\nabla \varphi_t^{GP}\|^2(\|p_1\Psi_t\|^2 - 1) = \|\nabla \varphi_t^{GP}\|^2\|q_1\Psi_t\|^2 \\ \leq \; & \|\nabla \varphi_t^{GP}\|^2\|\widehat{n}\,\Psi_t\|^2 \leq \|\nabla \varphi_t^{GP}\|^2\alpha(\Psi_t) . \end{aligned}$$

Choosing $\xi \leq \min\{\delta, 1/4, \beta, 1-\beta\}$ Lemma 5.4 follows.

□

5.2 Proof of Theorem 4.3 for $\beta < 1/3$

Lemma 4.7 with Lemma 5.1 and Lemma 5.4 gives

$$|\alpha'(\Psi_t)| \leq C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)(\sup_{0\leq s\leq t}\{\alpha(\Psi_s)\} + N^{-\xi}) \ . \tag{21}$$

We shall use a Gronwall argument to control $\alpha(\Psi_t)$: Consider the differential equation

$$\gamma_t' = C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)(\sup_{0\leq s\leq t}\{\gamma_s\} + N^{-\xi}) \ . \tag{22}$$

Since the right hand side of (22) is positive, the solution γ_t with $\gamma_0 = \alpha(\Psi_0)$ dominates $\alpha(\Psi_t)$. Moreover γ_t increases monotonously, thus $\sup_{0\leq s\leq t}\{\gamma_s\} = \gamma_t$ and

$$\gamma_t' = C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)(\gamma_t + N^{-\xi}) \ .$$

It follows that

$$\ln(\gamma_t + N^{-\xi}) = C\int_0^t (\|\varphi_s^{GP}\|_\infty + \|\nabla\varphi_s^{GP}\|_\infty)ds + K_N$$

where the integration constant K_N is such that $\gamma_0 = \alpha(\Psi_0)$, i.e.

$$\gamma_t = C_N \exp\left(C\int_0^t \|\varphi_s^{GP}\|_\infty + \|\nabla\varphi_s^{GP}\|_\infty ds\right) - N^{-\xi}$$

where $C_N = e^{K_N}$. Note that Lemma 2.4 implies with (11) that $\lim_{N\to\infty}\alpha(\Psi_0) = 0$, thus $\lim_{N\to\infty} C_N = 0$ and Theorem 4.3 follows for $0 < \beta < 1$.

□

6 The Gross Pitaevskii equation for $1/3 \leq \beta \leq 1$

6.1 Microscopic Structure

Definition 6.1 *Let $0 < \beta_1 < \beta_2 < 1$, $v^N_{\beta_2} \in \mathcal{V}_{\beta_2}$. We define the potential W_{β_1,β_2} via*

$$W^N_{\beta_1,\beta_2}(x) := \begin{cases} aN^{-1+3\beta_1}, & \text{for } RN^{-\beta_2} < x < R^N_{\beta_1,\beta_2}; \\ 0, & \text{else.} \end{cases}$$

Here $RN^{-\beta_2}$ is an upper bound on the radius of the support of $v^N_{\beta_2}$ (see Definition 4.2) and $R^N_{\beta_1,\beta_2}$ is the minimal value which ensures that the scattering length of $v^N_{\beta_2} - W^N_{\beta_1,\beta_2}$ is zero.

The respective zero energy scattering state shall be denoted by $f^N_{\beta_1,\beta_2}$, i.e.

$$\left(-\Delta + v^N_{\beta_2} - W^N_{\beta_1,\beta_2}\right) f^N_{\beta_1,\beta_2} = 0 \ ,$$

we shall also need

$$g^N_{\beta_1,\beta_2} = 1 - f^N_{\beta_1,\beta_2}$$

Lemma 6.2 *For any $0 < \beta_1 < \beta_2 \leq 1$, $v^N_{\beta_2} \in \mathcal{V}_{\beta_2}$*

(a)
$$\|g^N_{\beta_1,\beta_2}\| \leq \sqrt{8\pi} a N^{-1-\beta_1/2} \qquad \|g^N_{\beta_1,\beta_2}\|_1 \leq 16\pi a N^{-1-2\beta_1}$$

(b)
$$W^N_{\beta_1,\beta_2} f^N_{\beta_1,\beta_2} \in \mathcal{V}_{\beta_1}$$

(c) The operator $h := -\Delta + v^N_\beta - W^N_{\beta_1,\beta_2}$ is positive.

(d) For any $\beta < \gamma < 1$ let $B_\gamma := \{x \in \mathbb{R}^3 : |x| \leq N^{-\gamma}\}$. Then for any $\Psi \in \mathcal{D}(H)$
$$\|\mathbb{1}_{B_\gamma} \nabla \Psi\| + \langle \Psi, (v^N_\beta - W^N_{\beta_1,\beta_2})\Psi\rangle \geq 0$$

Proof: Let $j^N_{\beta_2}$ be the zero energy scattering state of the potential $\frac{1}{2} v^N_{\beta_2}$. Since $v^N_{\beta_2}$ is positive and has compact support of radius r_N it follows, that $1 > j^N_{\beta_2}(x) \geq 1 - a/(Nx)$for any $x \geq r_N$. Note, that the potential $W^N_{\beta_1,\beta_2}$ is zero inside the Ball around zero of radius $RN^{-\beta_2}$, hence $f^N_{\beta_1,\beta_2}$ is inside this Ball a multiple of $j^N_{\beta_2}$.

Let $R^N_{\beta_1,\beta_2}$ be such that $K^N_{\beta_1,\beta_2} f^N_{\beta_1,\beta_2}(x) = j^N_{\beta_2}(x)$ for any $x < N^{-\beta_1}$. By definition of the potential $W^N_{\beta_1,\beta_2}$ we have that $\partial_x f^N_{\beta_1,\beta_2}(x) \geq 0$: $R^N_{\beta_1,\beta_2}$ was defined to be the minimal value which ensures that the scattering length of $v^N_\beta - W^N_N$ is zero, thus $\partial_r f^N_N(r) \geq 0$ for $r < R^N_{\beta_1,\beta_2}$. It follows in particular that $f^N_{\beta_1,\beta_2} \leq 1$. Furthermore we have, since $W^N_{\beta_1,\beta_2}$ is positive, that $K^N_{\beta_1,\beta_2} \partial_r f^N_{\beta_1,\beta_2} \leq \partial_r j^N_{\beta_2}$ and $K^N_{\beta_1,\beta_2} f^N_{\beta_1,\beta_2} \leq j^N_{\beta_2}$.

Since $f^N_{\beta_1,\beta_2}(x) = 1$ for $x > 2N^{-\beta_1}$ and $\lim_{x\to\infty} j^N_{\beta_2}(x) = 1$ we get that $K^N_{\beta_1,\beta_2} \leq 1$, thus $1 > f^N_{\beta_1,\beta_2} \geq j^N_{\beta_2}$. Since $j^N_{\beta_2}(x) \geq 1 - a/(Nx)$ it follows that

$$|g^N_{\beta_1,\beta_2}(x)| \leq a/(Nx) \ . \tag{23}$$

Since $g^N_{\beta_1,\beta_2}(x) = 0$ for $x > 2N^{-\beta_1}$ it follows that

$$\begin{aligned} \|g^N_{\beta_1,\beta_2}\|^2 &\leq a^2 N^{-2} \int_0^{2N^{-\beta_1}} |x|^{-2} d^3x = 8N^{-\beta_1} \pi a^2 N^{-2} \\ \|g^N_{\beta_1,\beta_2}\|_1 &\leq aN^{-1} \int_0^{2N^{-\beta_1}} |x|^{-1} d^3x = 16 N^{-2\beta_1} \pi a N^{-1} \end{aligned}$$

which is (a).

Next we have to show that $W^N_{\beta_1,\beta_2} f^N_{\beta_1,\beta_2} \in \mathcal{V}_{\beta_1}$.

Since $K^N_{\beta_1,\beta_2} f^N_{\beta_1,\beta_2} > 1 - aN^{-1-\beta_1}$ on the support of $W^N_{\beta_1,\beta_2}$

$$\begin{aligned} \|W^N_{\beta_1,\beta_2} K^N_{\beta_1,\beta_2} f^N_{\beta_1,\beta_2}\|_1 &< \|W^N_{\beta_1,\beta_2} f^N_{\beta_1,\beta_2}\|_1 < \|W^N_{\beta_1,\beta_2}\|_1 \\ &< (1 - aN^{-1+\beta_1})^{-1} \|W^N_{\beta_1,\beta_2} K^N_{\beta_1,\beta_2} f^N_{\beta_1,\beta_2}\|_1 \\ &< (1 - aN^{-1+\beta_1})^{-1} \|W^N_{\beta_1,\beta_2} f^N_{\beta_1,\beta_2}\|_1 \ . \end{aligned} \tag{24}$$

Note also that $\|W^N_{\beta_1,\beta_2}K^N_{\beta_1,\beta_2}f^N_{\beta_1,\beta_2}\|_1 = a/N$: Read $\rho^N_{\beta_1,\beta_2} := W^N_{\beta_1,\beta_2}K^N_{\beta_1,\beta_2}f^N_{\beta_1,\beta_2}$ as a classical charge distribution which must compensate the charge a/N (recall that $K^N_{\beta_1,\beta_2}f^N_{\beta_1,\beta_2}(x) = 1 - a/(Nx)$ for $r_N < x < N^{-\beta}$) to get that the potential $\varphi_N \widehat{=} K^N_{\beta_1,\beta_2}f^N_{\beta_1,\beta_2}$ is zero outside the support of $W^N_{\beta_1,\beta_2}$. With (24) it follows that

$$\lim_{N\to\infty} N^{1-\beta_1}(\|W^N_{\beta_1,\beta_2}f^N_{\beta_1,\beta_2}\|_1 - a/N) < \infty \tag{25}$$

and again using (24)

$$\lim_{N\to\infty} N^{1-\beta_1}(\|W^N_{\beta_1,\beta_2}\|_1 - a/N) < \infty\ .$$

It follows that the support of $W^N_{\beta_1,\beta_2}$ is of order $N^{3\beta_1}$. Since $W^N_{\beta_1,\beta_2}f^N_{\beta_1,\beta_2}$ is spherically symmetric, positive and equal to zero for $x > R^N_{\beta_1,\beta_2}$ it follows that $W^N_{\beta_1,\beta_2}f^N_{\beta_1,\beta_2} \in \mathcal{W}_{\beta_1}$.

With (25) and using that $W^N_{\beta_1,\beta_2}$ is defined such that $\|W^N_{\beta_1,\beta_2}f^N_{\beta_1,\beta_2}\|_\infty \leq \|W^N_{\beta_1,\beta_2}\|_\infty = aN^{-1+3\beta_1}$ it follows that $W^N_{\beta_1,\beta_2}f^N_{\beta_1,\beta_2} \in \mathcal{V}_{\beta_1}$.

We show (c) by contradiction. Assume that h is not positive, thus it has a ground state χ. Since $f^N_{\beta_1,\beta_2}$ is by construction a positive function and so is the ground state χ it follows that $\int f^N_{\beta_1,\beta_2}(x)\chi^*(x)d^3x > 0$. But $f^N_{\beta_1,\beta_2}$ is the generalized eigenfunction of h with energy 0, so $\int f^N_{\beta_1,\beta_2}(x)\chi^*(x)d^3x = 0$ which leads to contradiction and (c) follows.

We shall also proof (d) by contradiction. Assume that there exists a $\chi \in L^2$ such that $\langle\nabla\chi, \mathbb{1}_{B_\gamma}\nabla\chi\rangle + \langle\chi, (v^N_\beta - W^N_{\beta_1,\beta_2})\chi\rangle < 0$. Since our potential is spherically symmetric we can assume without loss of generality that χ is spherically symmetric. Defining the function $\varphi(r) := \chi(r)$ for $r \leq N^{-\gamma}$ and $\varphi(r) = \chi(N^{-\gamma})$ for $r > N^{-\gamma}$ it follows that

$$\langle\varphi, h\varphi\rangle = \langle\nabla\chi, \mathbb{1}_{B_r}\nabla\chi\rangle + \langle\chi, (v^N_\beta - W^N_{\beta_1,\beta_2})\chi\rangle < 0\ .$$

This contradicts (c) and (d) follows.

□

6.2 Control of the kinetic energy for $\beta = 1$

Next we shall control the kinetic energy $\|\nabla_1\Psi\|$ for $\beta = 1$. Note that in this case, a relevant part of the kinetic energy is absorbed to form the microscopic structure. That part of the kinetic energy is concentrated around the scattering centers.

The microscopic structure can — as long as there are no three particle interactions — be controlled using Lemma 6.2. So we shall first cutoff three particle interactions without disturbing $\nabla_1\Psi$, i.e. we define a cutoff function which does not depend on x_1 and cuts off all parts of the wave function where two particles x_j, x_k with $j \neq k$, $j, k \neq 1$ come to close (R_1 given by Definition 6.3).

After that we shall subtract that part of the kinetic energy which is used to form the microscopic structure. The latter is concentrated around the scattering centra (i.e. on the set $\overline{\mathcal{S}}_j$ given by Definition 6.3).

Definition 6.3 *For any $j, k = \{1, \ldots, N\}$ let*

$$s_{j,k} := \{X \in \mathbb{R}^{3N} : |x_j - x_k| < N^{-26/27}\} \tag{26}$$

$$\overline{\mathcal{S}}_j := \bigcup_{k \neq j} s_{j,k} \qquad \mathcal{S}_j := \mathbb{R}^{3N} \backslash \overline{\mathcal{S}}_j \qquad \mathcal{R}_{j,k} := \bigcup_{l \neq j,k} s_{k,l} \qquad \mathcal{R}_{j,k} := \mathbb{R}^{3N} \backslash \overline{\mathcal{R}}_{j,k}$$

Proposition 6.4

$$\|\Psi_t - \mathbb{1}_{R_j}\Psi_t\| < CN^{-7/54} .$$

Proof:
Using Hölder and Sobolev we get

$$\begin{aligned}
\|\Psi_t - \mathbb{1}_{R_j}\Psi_t\| &= \|\Psi_t \mathbb{1}_{\overline{\mathcal{R}}_{j,k}}\|^2 \leq \|\mathbb{1}_{\overline{\mathcal{R}}_{j,k}}\|_{3/2} \, \|\Psi_t^2\|_3 = |\overline{\mathcal{R}}_{j,k}|^{2/3} \|\Psi_t\|_6^2 \\
&\leq (N-1)\|\nabla_1 \Psi_t\|^2 (NN^{-26/9})^{2/3} \leq N^{-7/27} \|\nabla_1 \Psi_t\|^2 .
\end{aligned}$$

Since $\|\nabla_1 \Psi_t\| < C$ the Proposition follows.

□

Lemma 6.5 *Let under the conditions of the Theorem $\beta \leq 1$. Then there exists a $\gamma > 0$ such that for any $t \in \mathbb{R}$*

$$\|\mathbb{1}_{\mathcal{S}_1} \nabla_1 q_1 \Psi_t\| < C(\alpha(\Psi_t) + \int_0^t \alpha(\Psi_s) ds + N^{-\gamma}) \tag{27}$$

$$\|\mathbb{1}_{\overline{\mathcal{R}}_1} \sqrt{v}_N (x_1 - x_2) \Psi_t\| < CN^{-1}(\alpha(\Psi_t) + \int_0^t \alpha(\Psi_s) ds + N^{-\gamma}) \tag{28}$$

Proof: Below we shall use from time to time that for any $f \in L^2$, any $g \in L^1$ and any normalized Ψ, χ

$$\|f(x_1 - x_2) p_1 \Psi\|^2 = \langle \Psi p_1 f^2 (x_1 - x_2) p_1 \Psi \rangle \leq \|f^2\|_1 \|\varphi^{GP}\|_\infty^2$$

and

$$\langle \chi p_1 g(x_1 - x_2) p_1 \Psi \rangle \leq \|g\|_1 \|\varphi^{GP}\|_\infty^2$$

Thus

$$\|f(x_1 - x_2) p_1\|_{op} \leq \|f\| \|\varphi^{GP}\|_\infty \tag{29}$$

and

$$\|p_1 g(x_1 - x_2) p_1\|_{op} \leq \|g\|_1 \|\varphi^{GP}\|_\infty^2 , \tag{30}$$

where $\| \cdot \|_{op}$ stands for the operator norm

$$\|A\|_{op} := \inf_{\|\Psi\|=1} \|A\Psi\| .$$

Let us now prove Lemma 6.5. Recall (18)

$$\begin{aligned}
& C(N^{-\delta}+N^{-1/4}+\sup_{0\leq s\geq t}\{\alpha(\Psi_s)\}) \\
\geq\ & \|\nabla_1\Psi_t\|^2-\|\nabla\varphi_t^{GP}\|^2+\left\langle\Psi_t,\left((N-1)v_1^N(x_1-x_2)-a|\varphi_t^{GP}|^2(x_1)\right)\Psi_t\right\rangle \\
=\ & \langle\nabla_1\Psi_t,\mathbb{1}_{\mathcal{S}_1}\nabla_1\Psi_t\rangle+\langle\nabla_1\Psi_t,\mathbb{1}_{\overline{\mathcal{S}}_1}\nabla_1\Psi_t\rangle-E_{kin}^{GP} \\
& +\langle\Psi_t,\sum_{j\neq 1}\mathbb{1}_{\mathcal{R}_{1,j}}\left(v_1^N(x_1-x_j)-W_{\beta,1}^N(x_1-x_j)\right)\Psi_t\rangle \\
& +\langle\Psi_t,\left(\sum_{j\neq 1}\mathbb{1}_{\mathcal{R}_{1,j}}W_{\beta,1}^N(x_1-x_j)-a|\varphi_t^{GP}(x_1)|^2\right)\Psi_t\rangle \\
& +\langle\Psi_t,\sum_{j\neq 1}\mathbb{1}_{\overline{\mathcal{R}}_{1,j}}v_1^N(x_1-x_j)\Psi_t\rangle\ .
\end{aligned}$$

By definition of the set $\mathcal{S}_1$ the support of the potentials $v_1^N(x_1-x_j)$ and $W_{\beta,1}^N(x_1-x_j)$ are subsets of $\overline{\mathcal{S}}_1:=\mathbb{R}^{3N}\backslash\mathcal{S}_1$. Furthermore we have by definition of the set $\mathcal{R}_{1,j}$ that the support of the potentials $\mathbb{1}_{\mathcal{R}_{1,j}}\left(v_1^N(x_1-x_j)-W_{\beta,1}^N(x_1-x_j)\right)$ are pairwise disjoint for different j. It follows with Lemma 6.2 (d) that

$$\langle\nabla_1\Psi_t,\mathbb{1}_{\overline{\mathcal{S}}_1}\nabla_1\Psi_t\rangle+\langle\Psi_t,\sum_{j\neq 1}\mathbb{1}_{\mathcal{R}_{1,j}}\left(v_1^N(x_1-x_j)-W_{\beta,1}^N(x_1-x_j)\right)\Psi_t\rangle$$

is positive and

$$\begin{aligned}
& \langle\nabla_1\Psi_t,\mathbb{1}_{\overline{\mathcal{S}}_1}\nabla_1\Psi_t\rangle-E_{kin}^{GP}+\langle\Psi_t,\left(\sum_{j\neq 1}\mathbb{1}_{\mathcal{R}_{1,j}}W_{\beta,1}^N(x_1-x_j)-a|\varphi_t^{GP}(x_1)|^2\right)\Psi_t\rangle \\
& +\langle\Psi_t,\sum_{j\neq 1}\mathbb{1}_{\overline{\mathcal{R}}_{1,j}}v_1^N(x_1-x_j)\Psi_t\rangle\leq C(N^{-\delta}+N^{-1/4}+\sup_{0\leq s\leq t}\{\alpha(\Psi_s)\})\ . \qquad (31)
\end{aligned}$$

For the last summand in the first line we have using positivity of $W_{\beta,1}^N$

$$
\begin{aligned}
& \langle\Psi_t, \left(\sum_{j\neq 1}\mathbb{1}_{\mathcal{R}_{1,j}}W_{\beta,1}^N(x_1-x_j)-a|\varphi_t^{GP}(x_1)|^2\right)\Psi_t\rangle \\
= & \langle\Psi_t, p_1p_2\left(\sum_{j\neq 1}W_{\beta,1}^N(x_1-x_j)-a|\varphi_t^{GP}(x_1)|^2\right)p_1p_2\Psi_t\rangle \\
& -\langle\Psi_t, p_1p_2\sum_{j\neq 1}\mathbb{1}_{\overline{\mathcal{R}}_{1,j}}W_{\beta,1}^N(x_1-x_j)p_1p_2\Psi_t\rangle \\
& +2\Re\left(\langle(1-p_1p_2)\Psi_t, \left(\sum_{j\neq 1}W_{\beta,1}^N(x_1-x_j)-a|\varphi_t^{GP}(x_1)|^2\right)p_1p_2\Psi_t\rangle\right) \\
& +2\Re\left(\langle(1-p_1p_2)\Psi_t, \sum_{j\neq 1}\mathbb{1}_{\overline{\mathcal{R}}_{1,j}}W_{\beta,1}^N(x_1-x_j)p_1p_2\Psi_t\rangle\right) \\
& +\langle(1-p_1p_2)\Psi_t, \sum_{j\neq 1}\mathbb{1}_{\mathcal{R}_{1,j}}W_{\beta,1}^N(x_1-x_j)\langle(1-p_1p_2)\Psi_t\rangle \\
& -\langle(1-p_1p_2)\Psi_t, a|\varphi_t^{GP}(x_1)|^2\langle(1-p_1p_2)\Psi_t\rangle \\
=: & \sum_{j=1}^{6}S_j;
\end{aligned}
$$

We already got bounds on S_1, S_3 and S_6: All these terms appeared in (19) above and could be estimated by the right hand side of Lemma 5.4. $S_5>0$ since $W_{1,\beta}^N$ is positive. For S_2 we have

$$
\begin{aligned}
& \left|\langle\Psi_t, p_1p_2\sum_{j\neq 1}\mathbb{1}_{\overline{\mathcal{R}}_{1,j}}W_{\beta,1}^N(x_1-x_j)p_1p_2\Psi_t\rangle\right| \\
\leq\ & (N-1)\|p_1W_{\beta,1}^N(x_1-x_2)p_1\|_{op}\ \|\mathbb{1}_{\overline{\mathcal{R}}_{1,j}}p_2\Psi_t\|^2 \\
\leq\ & (N-1)\|p_1W_{\beta,1}^N(x_1-x_2)p_1\|_{op}\left(\|\mathbb{1}_{\overline{\mathcal{R}}_{1,j}}\Psi_t\|+\|\mathbb{1}_{s_{2,j}}p_2\Psi_t\|\right)^2
\end{aligned}
$$

which is in view of Proposition 6.4 bounded by the right hand of (27).

For S_4 we have

$$
\begin{aligned}
& 2\left|\Re\left(\langle(1-p_1p_2)\Psi_t, \sum_{j\neq 1}\mathbb{1}_{\overline{\mathcal{R}}_{1,j}}W_{\beta,1}^N(x_1-x_j)p_1p_2\Psi_t\rangle\right)\right| \qquad (32) \\
\leq\ & 2(N-1)\|\sqrt{W_{\beta,1}^N}(x_1-x_2)(1-p_1p_2)\Psi_t\|\ \|\mathbb{1}_{\overline{\mathcal{R}}_{1,2}}\sqrt{W_{\beta,1}^N}(x_1-x_2)p_1p_2\Psi_t\|
\end{aligned}
$$

Using Hölder and Sobolev we have

$$\begin{aligned}\|\sqrt{W^N_{\beta,1}}(x_1-x_2)\Psi_t\|^2 &\leq \|W^N_{\beta,1}\|_{3/2}\ \|\Psi\|_6^2\\ \leq \left(\int |W^N_{\beta,1}(x)|^{3/2}d^3x\right)^{2/3}\ \|\nabla\Psi\|^2 &\leq C(N^{-3/2+3\beta/2})^{2/3}=CN^{-1+\beta}\ .\end{aligned}$$

Since

$$\begin{aligned}&\|\mathbb{1}_{\overline{\mathcal{R}}_{1,2}}\sqrt{W^N_{\beta,1}}(x_1-x_2)p_1p_2\Psi_t\|^2 \leq \|p_2\mathbb{1}_{\overline{\mathcal{R}}_{1,2}}p_2\|_{op}\|\sqrt{W^N_{\beta,1}}(x_1-x_2)p_1\Psi_t\|^2\\ \leq\ & |\overline{\mathcal{R}}_{1,2}|CN^{-1}\leq CNN^{-26/9}N^{-1}=CN^{-26/9}\end{aligned}$$

it follows with (32) that S_4 is bounded by the right hand side of (27). Hence

$$\begin{aligned}&\langle\nabla_1\Psi_t,\mathbb{1}_{\overline{\mathcal{S}}_1}\nabla_1\Psi_t\rangle - E^{GP}_{kin}+\langle\Psi_t,\sum_{j\neq 1}\mathbb{1}_{\overline{\mathcal{R}}_{1,j}}v_1^N(x_1-x_j)\Psi_t\rangle\\ \leq\ & C(N^{-\delta}+N^{-1/4}+\sup_{0\leq s\leq t}\{\alpha(\Psi_s)\})\ .\end{aligned}\tag{33}$$

For the first summand in (33) we can write

$$\begin{aligned}\|\mathbb{1}_{\mathcal{S}_1}\nabla_1\Psi_t\|^2 &\geq \|\mathbb{1}_{\mathcal{S}_1}\nabla_1p_1\Psi_t\|^2+\|\mathbb{1}_{\mathcal{S}_1}\nabla_1q_1\Psi_t\|^2-2|\langle\nabla_1q_1\Psi_t,\nabla_1p_1\Psi_t\rangle|\\ &\quad -2|\langle\nabla_1q_1\Psi_t,\mathbb{1}_{\overline{\mathcal{S}}_1}\nabla_1p_1\Psi_t\rangle|\\ &\geq \|\nabla_1p_1\Psi_t\|^2+\|\mathbb{1}_{\mathcal{S}_1}\nabla_1q_1\Psi_t\|^2-\|\mathbb{1}_{\overline{\mathcal{S}}_1}\nabla_1p_1\Psi_t\|^2\\ &\quad +\langle q_1\Psi_t,\Delta_1p_1\Psi_t\rangle-\|\nabla_1q_1\Psi_t\|\ \|\mathbb{1}_{\overline{\mathcal{S}}_1}\|_1^{1/2}\ \|\nabla_1\varphi_t^{GP}\|_\infty\\ &\geq \|\nabla\varphi^{GP}\|\ \|p_1\Psi_t\|+\|\mathbb{1}_{\mathcal{S}_1}\nabla_1q_1\Psi_t\|^2\\ &\quad -\|\mathbb{1}_{\overline{\mathcal{S}}_1}\|_1^2\ \|\nabla_1\varphi_t^{GP}\|_\infty^2-\|q_1\Psi_t\|\ \|\Delta_1\varphi_t^{GP}\|_\infty\ \|p_1\Psi_t\|\\ &\quad -(\|\nabla_1\Psi_t\|+\|\nabla_1p_t\Psi_t\|)\ \|\mathbb{1}_{\overline{\mathcal{S}}_1}\|_1^{1/2}\ \|\nabla_1\varphi_t^{GP}\|_\infty\ .\end{aligned}$$

Since

$$\|\mathbb{1}_{\overline{\mathcal{S}}_1}\|_1\leq N|s_{1,2}|=4/3\pi N^{-17/9}\tag{34}$$

we can find a $\gamma>0$ such that

$$\begin{aligned}&\|\mathbb{1}_{\mathcal{S}_1}\nabla_1q_1\Psi_t\|^2+\langle\Psi_t,\mathbb{1}_{\overline{\mathcal{R}}_1}\sum_{j\neq 1}v_1^N(x_1-x_j)\Psi_t\rangle\\ \leq\ & E_{kin}(1-\|p_t\Psi_t\|^2)+C(\alpha(\Psi_0)+\alpha(\Psi_t))+C\int_0^t\alpha(\Psi_s)ds+CN^{-\gamma}\ .\end{aligned}$$

Using that $1-\|p_t\Psi_t\|^2=\|q_t\Psi_t\|^2<\alpha(\Psi)$ and that both summands are positive the Lemma follows.

□

6.3 Redefinition of α for $1/3 < \beta \leq 1$

As mentioned in the introduction one has to control the microscopic structure of Ψ when β increases. On the technical level that means, that for $\beta > 1/3$ the α'_1 and for $\beta = 1$ the α'_2 can't be controlled. We have to equip the $\alpha_{1/2}$ with the respective microscopic structure. We shall do that by adding the functions $\lambda_{1,2}$ to $\alpha_{1/2}$ and $\lambda'_{1,2}$ to $\alpha'_{1/2}$ in such a way, that $\lambda'_{1,2}(\Psi_t)$ is the time dericative $\lambda_{1,2}(\Psi_t)$ if Ψ_t solves the Schrödinger equation and $\alpha_{1,2}+\lambda_{1,2}$ becomes controllable.

First note that we can replace in the estimate of the second term in Lemma 5.2 (a) $\|\nabla_1 q_1 \Psi_t\|$ by $\|\mathbb{1}_{\mathcal{S}_1}\nabla_1 q_1\Psi_t\|$:

Lemma 6.6 *Under the conditions of Lemma 5.2 we have for* $0 < \beta < 1$

$$\begin{aligned}|\langle\Psi_t, p_1q_2\widehat{m}^{1/2}h_{1,2}\widehat{m}^{1/2}q_1q_2\Psi_t\rangle|\\ \leq C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)(\alpha(\Psi) + N^{-\gamma} + \|\mathbb{1}_{\mathcal{S}_1}\nabla_1 q_1\Psi_t\|^2)\end{aligned}$$

The proof shall be given in the Appendix.

Definition 6.7 *Let* $v_1^N \in \mathcal{V}_1$.
We define

$$\lambda_2(\Psi) := N(N-1)\Im\left(\left\langle\Psi, g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\right\rangle\right)$$

and

$$\begin{aligned}\lambda'_2(\Psi) := {} & N(N-1)\Im\left(\left\langle\Psi, \left[H, g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\right]\Psi\right\rangle\right)\\ & -N(N-1)\Im\left(\left\langle\Psi, g^N_{8/9,1}(x_1-x_2)\left[H^{GP},(\widehat{n}-\widehat{n}_1)p_1q_2\right]\Psi\right\rangle\right) .\end{aligned}$$

Lemma 6.8 *There exists a* $\gamma > 0$ *such that*

(a) For any solution of the Schödinger equation $\Psi_t \in L^2(\mathbb{R}^{3N}\to\mathbb{C})$

$$i\frac{d}{dt}\lambda_2(\Psi_t) = \lambda'_2(\Psi_t)$$

(b) There exist a $C<\infty$ *such that for any* $\Psi \in L^2(\mathbb{R}^{3N}\to\mathbb{C})$

$$|\lambda'_2(\Psi) - \alpha'_2(\Psi)| \leq C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)\left(N^{-\gamma} + (\ln N)^{1/3}\alpha(\Psi)\right) . \tag{35}$$

(c)

$$|\lambda_2(\Psi)| \leq CN^{-\gamma}\|\varphi_t^{GP}\|_\infty$$

Proof: (a) follows as above, using that $\frac{d}{dt}\widehat{m} = -[H^{GP},\widehat{m}]$.
For (c) we have with Lemma 2.3

$$|\lambda_2(\Psi)| \leq N^2\|g^N_{8/9,1}\|\,\|\varphi_t^{GP}\|_\infty\,\|(\widehat{n}-\widehat{n}_1)q_2\Psi\| \leq CN^{-4/9}\|\varphi_t^{GP}\|_\infty$$

For (b) we have since

$$
\begin{aligned}
& [H, g^N_{8/9,1}(x_1-x_2)] = [H, f^N_{8/9,1}(x_1-x_2)] = -[\Delta_1+\Delta_2, f^N_{8/9,1}(x_1-x_2)] \\
= \; & (\Delta_1+\Delta_2) f^N_{8/9,1}(x_1-x_2) + (\nabla_1 f^N_{8/9,1}(x_1-x_2))\nabla_1 + (\nabla_2 f^N_{8/9,1}(x_1-x_2))\nabla_2 \\
= \; & (v^N_\beta - W^N_{8/9,1}) f^N_{8/9,1}(x_1-x_2) + (\nabla_1 g^N_{8/9,1}(x_1-x_2))\nabla_1 + (\nabla_2 g^N_{8/9,1}(x_1-x_2))\nabla_2
\end{aligned}
$$

that

$$
\begin{aligned}
\lambda'_2(\Psi) \; = \; & N(N-1)\Im\left(\left\langle\Psi, \left[(H-H^{GP}), g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\right]\Psi\right\rangle\right) \\
& + N(N-1)\Im\big(\langle\Psi, \big((v^N_\beta - W^N_{8/9,1}) f^N_{8/9,1}(x_1-x_2) \\
& + (\nabla_1 g^N_{8/9,1}(x_1-x_2))\nabla_1 + (\nabla_2 g^N_{8/9,1}(x_1-x_2))\nabla_2\big)(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\rangle\big) \; .
\end{aligned}
$$

It follows that

$$
\begin{aligned}
\lambda'_2(\Psi) - \alpha'_2(\Psi) \; = \; & N(N-1)\Im\left(\left\langle\Psi, \left[-a_N\sum_{j=1}^N |\varphi^{GP}_t|^2(x_j), g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\right]\Psi\right\rangle\right) \\
& + N(N-1)\Im\left(\left\langle\Psi, W^N_{8/9,1} g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\right\rangle\right) \\
& + N(N-1)\Im\big(\langle\Psi, \big((\nabla_1 g^N_{8/9,1}(x_1-x_2))\nabla_1 \\
& + (\nabla_2 g^N_{8/9,1}(x_1-x_2))\nabla_2\big)(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\rangle\big) \\
& - N(N-1)\Im\left(\left\langle\Psi, g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\sum_{j<k} v^N_\beta(x_j-x_k)\Psi\right\rangle\right) \\
& + N(N-1)\Im\left(\left\langle\Psi, \sum_{j=1}^2\sum_{k=3}^N v^N_\beta(x_j-x_k) g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\right\rangle\right) \\
& + N(N-1)\Im\left(\left\langle\Psi, \sum_{2<j<k}^N v^N_\beta(x_j-x_k) g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\right\rangle\right) \; .
\end{aligned}
$$

Using symmetry of Ψ and $\nabla_1 g^N_{\beta_1,\beta_2} = -\nabla_2 g^N_{\beta_1,\beta_2}$

$$\begin{aligned}
&\lambda_2'(\Psi) - \alpha_2'(\Psi) \\
= \quad & N(N-1)\Im\left(\left\langle \Psi, \left[-a_N \sum_{j=1}^N |\varphi_t^{GP}|^2(x_j), g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\right]\Psi\right\rangle\right) \\
&+N(N-1)\Im\left(\left\langle \Psi, W^N_{8/9,1} f^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\right\rangle\right) \\
&-N(N-1)\Im\left(\left\langle \Psi, (\nabla_2 g^N_{8/9,1}(x_1-x_2))\nabla_1 p_1q_2(\widehat{n}-\widehat{n}_1)\Psi\right\rangle\right) \\
&-N(N-1)\Im\left(\left\langle \Psi, (\nabla_1 g^N_{8/9,1}(x_1-x_2))\nabla_2 p_1q_2(\widehat{n}-\widehat{n}_1)\Psi\right\rangle\right) \\
&-N(N-1)\Im\left(\left\langle \Psi, g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2 v^N_\beta(x_1-x_2)\Psi\right\rangle\right) \\
&-\frac{N!}{(N-3)!}\Im\left(\left\langle \Psi, g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2 v^N_\beta(x_2-x_3)\Psi\right\rangle\right) \\
&-\frac{N!}{(N-3)!}\Im\left(\left\langle \Psi, g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2 v^N_\beta(x_1-x_3)\Psi\right\rangle\right) \\
&-\frac{N!}{(N-4)!}\Im\left(\left\langle \Psi, g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2 v^N_\beta(x_3-x_4)\Psi\right\rangle\right) \\
&+\frac{N!}{(N-3)!}\Im\left(\left\langle \Psi, v^N_\beta(x_2-x_3) g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\right\rangle\right) \\
&+\frac{N!}{(N-3)!}\Im\left(\left\langle \Psi, v^N_\beta(x_1-x_3) g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\right\rangle\right) \\
&+\frac{N!}{(N-4)!}\Im\left(\left\langle \Psi, v^N_\beta(x_3-x_4) g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\right\rangle\right) \\
=: \quad & \sum_{j=0}^{10} S_j \; . \qquad (36)
\end{aligned}$$

For the first summand we have

$$|S_0| \quad \leq \quad 2N^2 a \|\varphi_t^{GP}\|^3_\infty \, \|g^N_{8/9,1}\| \, \|(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\| \; .$$

With Lemma 6.5 it follows that $|S_0|$ is bounded by the right hand side of (35).

Using as above (see proof of Lemma 5.1) that $\Im(\langle \Psi, A\Psi\rangle) = -\Im(\langle \Psi, A^t\Psi\rangle)$ for any operator A and that Ψ is symmetric (note that $p_1q_2v^N_\beta(x_1-x_2)q_1p_2$ is invariant under adjunction plus exchange of the variable x_1 and x_2) and Lemma 2.3 (d) we get for S_1

$$\begin{aligned}
|S_1| \quad \leq \quad & N(N-1)\left|\Im\left(\left\langle \Psi, p_1p_2 W^N_{8/9,1} f^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\right\rangle\right)\right| \\
&+N(N-1)\left|\Im\left(\left\langle \Psi, q_1q_2 W^N_{8/9,1} f^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2\Psi\right\rangle\right)\right|
\end{aligned}$$

Since $W^N_{8/9,1} f^N_{8/9,1} \in \mathcal{V}_{\beta_2}$ (see Lemma 6.2 (b)) it follows with Lemma 6.6 that

$$|S_1| \leq C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)(\alpha(\Psi) + \|\mathbb{1}_{\mathcal{S}_1}\nabla_1 q_1\Psi_t\| + N^{-\xi}) \; .$$

With Lemma 6.5 it follows that $|S_1|$ is bounded by the right hand side of (35).

For S_2 and S_3 we get integrating by parts

$$\begin{aligned} S_2+S_3 &= N(N-1)\Im\left(\left\langle \nabla_2\Psi, (g^N_{8/9,1}(x_1-x_2))\nabla_1 p_1 q_2(\widehat{n}-\widehat{n}_1)\Psi\right\rangle\right) \\ & N(N-1)\Im\left(\left\langle (q_1q_2+1-q_1q_2)\nabla_1\Psi, (g^N_{8/9,1}(x_1-x_2))\nabla_2 p_1 q_2(\widehat{n}-\widehat{n}_1)\Psi\right\rangle\right) \\ & +2N(N-1)\Im\left(\left\langle (q_1q_2+1-q_1q_2)\Psi, (g^N_{8/9,1}(x_1-x_2))\nabla_1\nabla_2 p_1 q_2(\widehat{n}-\widehat{n}_1)\Psi\right\rangle\right) \ . \end{aligned}$$

Thus

$$\begin{aligned} |S_2+S_3| &\leq N(N-1)\|\nabla_2\Psi\|\ \|g^N_{8/9,1}\|\ \|\nabla_1\varphi^{GP}_t\|_\infty\ \|p_1q_2(\widehat{n}-\widehat{n}_1)\Psi\| \\ &+N(N-1)\|q_1\nabla_2 q_2(\widehat{n}_2-\widehat{n}_3)\Psi\|\ \|g^N_{8/9,1}\|\ \|\varphi^{GP}_t\|_\infty\ \|\nabla_2 p_1 q_2(\widehat{n}-\widehat{n}_1)\Psi\| \\ &+N(N-1)\|\nabla_1\Psi\|\ \|g^N_{8/9,1}\|_1\ \|\varphi^{GP}_t\|^2_\infty\ \|\widehat{n}-\widehat{n}_1\|_{op}\ \|\nabla_2 q_2\Psi\| \\ &+2N(N-1)\|q_1q_2(\widehat{n}_2-\widehat{n}_3)\Psi\|\ \|g^N_{8/9,1}\|_1\ \|\varphi^{GP}_t\|_\infty\ \|\nabla_1\varphi^{GP}_t\|_\infty\ \|\nabla_2 p_1 q_2(\widehat{n}-\widehat{n}_1)\Psi\| \\ &+2N(N-1)\|\Psi\|\ \|g^N_{8/9,1}\|_1\ \|\varphi^{GP}_t\|_\infty\ \|\nabla_1\varphi^{GP}_t\|_\infty\ \|\widehat{n}-\widehat{n}_1\|_{op}\ \|\nabla_2 q_2\Psi\| \ . \end{aligned}$$

With Lemma 6.5 it follows that $|S_2+S_3|$ is bounded by the right hand side of (35).

For S_4 we have

$$|S_4| \leq N(N-1)\|\Psi\|\ \|g^N_{8/9,1}(x_1-x_2)\|\ \|\varphi^{GP}_t\|_\infty\ \|\|\sqrt{v^N_\beta}\|\ \|\sqrt{v^N_\beta}\Psi\| + a\|\varphi^{GP}\|_\infty\ \|\Psi\|) \ .$$

With Lemma 6.5 it follows that $|S_4|$ is bounded by the right hand side of (35).

For S_5 we have using $q_2 = 1-p_2$

$$\begin{aligned} |S_5| &\leq \frac{N!}{(N-3)!}\left|\Im\left(\left\langle (p_1+q_1)\sqrt{v}^N_\beta(x_2-x_3)\Psi, g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1\sqrt{v}^N_\beta(x_2-x_3)\Psi\right\rangle\right)\right| \\ &+\frac{N!}{(N-3)!}\left|\Im\left(\left\langle \Psi, (q_1q_2+1-q_1q_2)g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1p_2 v^N_\beta(x_2-x_3)\Psi\right\rangle\right)\right| \end{aligned}$$

For the first summand we have

$$\begin{aligned} & \frac{N!}{(N-3)!}\left|\Im\left(\left\langle (p_1+q_1)\sqrt{v}^N_\beta(x_2-x_3)\Psi, g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1\sqrt{v}^N_\beta(x_2-x_3)\Psi\right\rangle\right)\right| \\ \leq\ & \frac{N!}{(N-3)!}\|\sqrt{v^N_\beta(x_2-x_3)}\Psi\|\ \|(\widehat{n}_1-\widehat{n}_2)q_1q_2\|_{op}\|g^N_{8/9,1}\|_1\ \|\varphi^{GP}_t\|^2_\infty\ \|\sqrt{v^N_\beta(x_2-x_3)}\Psi\| \\ & +\frac{N!}{(N-3)!}\|(\widehat{n}_1-\widehat{n}_2)q_1\sqrt{v^N_\beta(x_2-x_3)}\Psi\| \\ & \qquad \|g^N_{8/9,1}\|\ \|\varphi^{GP}_t\|_\infty\ \|\sqrt{v^N_\beta(x_2-x_3)}\Psi\| \end{aligned}$$

which is due to Lemma 6.5 and Lemma 2.3 bounded by the right hand side of

(35). For the second summand we have in view of Lemma 2.3 (d)

$$\begin{aligned}
&\frac{N!}{(N-3)!}\left|\Im\left(\left\langle\Psi,(q_1q_2+1-q_1q_2)g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1p_2v^N_\beta(x_2-x_3)\Psi\right\rangle\right)\right| \\
\leq\ &\frac{N!}{(N-3)!}\|(\widehat{n}_1-\widehat{n}_2)q_1q_2\Psi\|\ \|g^N_{8/9,1}\|\ \|\varphi^{GP}_t\|^2_\infty\ \|\sqrt{v^N_\beta}\|\ \|\sqrt{v^N_\beta(x_2-x_3)}\Psi\| \\
&+\frac{N!}{(N-3)!}\|g^N_{8/9,1}\|_1\ \|\varphi^{GP}_t\|^2\ \|\widehat{n}-\widehat{n}_1\|_{op}\ \|\varphi^{GP}_t\|_\infty\ \|\sqrt{v^N_\beta}\|\ \|\sqrt{v^N_\beta}(x_2-x_3)\Psi\|\ .
\end{aligned}$$

With Lemma 6.5 it follows that $|S_5|$ is bounded by the right hand side of (35).

Similarly we get for S_6 using Lemma 2.3 (d)

$$\begin{aligned}
|S_6|\ =\ &\frac{N!}{(N-3)!}\left|\Im\left(\left\langle\Psi,(q_1q_2+1-q_1q_2)g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1q_2v^N_\beta(x_1-x_3)\Psi\right\rangle\right)\right| \\
\leq\ &\frac{N!}{(N-3)!}\|(\widehat{n}_1-\widehat{n}_2)q_1q_2\Psi\|\ \|g^N_{8/9,1}\|\ \|\varphi^{GP}_t\|^2_\infty\ \|\sqrt{v^N_\beta(x_1-x_3)}\|\ \|\sqrt{v^N_\beta(x_1-x_3)}\Psi\| \\
&+\|(\widehat{n}_1-\widehat{n}_2)q_1q_2\Psi\|\ \|g^N_{8/9,1}\|\ \|\varphi^{GP}_t\|_\infty\ a/N\|\varphi^{GP}_t\|\ \|\Psi\| \\
&+\|g^N_{8/9,1}\|_1\ \|\varphi^{GP}_t\|^2\ \|\widehat{n}-\widehat{n}_1\|_{op}\ \|\varphi^{GP}_t\|_\infty\ \|\sqrt{v^N_\beta}\|\ \|\sqrt{v^N_\beta}(x_1-x_3)\Psi\|\ .
\end{aligned}$$

With Lemma 6.5 it follows that $|S_6|$ is bounded by the right hand side of (35).

For S_7+S_{10} we use (17) to get

$$\begin{aligned}
S_7+S_{10}\ =\ &-\frac{N!}{(N-4)!}\Im\left(\left\langle\Psi,g^N_{8/9,1}(x_1-x_2)Qv^N_\beta(x_3-x_4)\Psi\right\rangle\right) \\
&+\frac{N!}{(N-4)!}\Im\left(\left\langle\Psi,g^N_{8/9,1}(x_1-x_2)v^N_\beta(x_3-x_4)Q\Psi\right\rangle\right)
\end{aligned}$$

with

$$Q=(\widehat{n}-\widehat{n}_2-\widehat{n}_1+\widehat{n}_3)p_1q_2p_3p_4+(\widehat{n}-2\widehat{n}_1+\widehat{n}_2)(p_1q_2p_3q_4+p_1q_2q_3p_4)\ .$$

Since $\sqrt{k}-\sqrt{k-2}-\sqrt{k-1}+\sqrt{k-3}<Ck^{-3/2}$ and $\sqrt{k}-2\sqrt{k-1}+\sqrt{k-2}<Ck^{-3/2}$ it follows that

$$Q<N^{-2}\widehat{n}^{-3/2}(p_1q_2p_3p_4+p_1q_2p_3q_4+p_1q_2q_3p_4)\ .$$

It follows using symmetry and Lemma 2.3 that

$$\begin{aligned}
&|S_7+S_{10}|\\
\leq\ & N^2\left|\Im\left(\left\langle\Psi,q_1q_2\widehat{n}_1^{-1}g^N_{8/9,1}(x_1-x_2)\widehat{n}^{-1/2}(p_1q_2p_3p_4+2p_1q_2p_3q_4)v^N_\beta(x_3-x_4)\Psi\right\rangle\right)\right|\\
&+N^2\left|\Im\left(\left\langle\Psi,(1-q_1q_2)g^N_{8/9,1}(x_1-x_2)\widehat{n}^{-3/2}(p_1q_2p_3p_4+2p_1q_2p_3q_4)v^N_\beta(x_3-x_4)\Psi\right\rangle\right)\right|\\
&+N^2\left|\Im\left(\left\langle\Psi,q_1q_2v^N_\beta(x_3-x_4)\widehat{n}_1^{-1}g^N_{8/9,1}(x_1-x_2)\widehat{n}^{-1/2}(p_1q_2p_3p_4+2p_1q_2p_3q_4)\Psi\right\rangle\right)\right|\\
&+N^2\left|\Im\left(\left\langle\Psi,(1-q_1q_2)g^N_{8/9,1}(x_1-x_2)v^N_\beta(x_3-x_4)\widehat{n}^{-3/2}(p_1q_2p_3p_4+2p_1q_2p_3q_4)\Psi\right\rangle\right)\right|\\
\leq\ & 3N^2\|\widehat{n}_1^{-1}q_1q_2\Psi\|\;\|g^N_{8/9,1}\|\;\|\varphi^{GP}_t\|^2_\infty\;\|\sqrt{v^N_\beta}\|\;\|\sqrt{v^N_\beta}\Psi\|\\
&+3N^2\|g^N_{8/9,1}\|_1\;\|\varphi^{GP}_t\|^3_\infty\;\|\sqrt{v^N_\beta}\|\;\|\widehat{n}^{-3/2}q_2\sqrt{v^N_\beta}(x_3-x_4)\Psi\|\\
&+3N^2\sum_{j=1}^3\|\sqrt{v^N_\beta}\widehat{n}_j^{-1}q_1q_2\Psi\|\;\|g^N_{8/9,1}\|\;\|\varphi^{GP}_t\|^2_\infty\;\|\sqrt{v^N_\beta}\|\\
&+3N^2\|\sqrt{v^N_\beta}(x_3-x_4)\Psi\|\;\|g^N_{8/9,1}\|_1\;\|\varphi^{GP}_t\|^3_\infty\;\|\sqrt{v^N_\beta}\|\;\|\widehat{n}^{-3/2}q_2\Psi\|\;.
\end{aligned}$$

With Lemma 6.5 it follows that $|S_7+S_{10}|$ is bounded by the right hand side of (35).

For S_8 and S_9 note first, that

$$\begin{aligned}
&\left|\frac{N!}{(N-3)!}\Im\left(\left\langle\Psi,v^N_\beta(x_2-x_3)g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1p_2\Psi\right\rangle\right)\right|\\
\leq\ & CN^2\left|\left\langle\Psi,p_1v^N_\beta(x_2-x_3)g^N_{8/9,1}(x_1-x_2)\widehat{n}^{-1/2}p_1p_2\Psi\right\rangle\right|\\
&+CN^2\left|\left\langle\Psi,q_1v^N_\beta(x_2-x_3)g^N_{8/9,1}(x_1-x_2)\widehat{n}^{-1/2}p_1p_2\Psi\right\rangle\right|\\
\leq\ & CN^2\|\sqrt{v^N_\beta}(x_2-x_3)\Psi\|\;\|\varphi^{GP}_t\|^2\;\|g^N_{8/9,1}\|_1N^{1/2}\|\varphi^{GP}_t\|\;\|\sqrt{v^N_\beta}(x_2-x_3)\|\\
&+\sum_{j=1}^3CN^2\|\widehat{n}_j^{-1/2}v^N_\beta(x_2-x_3)q_1\Psi\|\;\|\varphi^{GP}_t\|\;\|g^N_{8/9,1}\|\;\|\varphi^{GP}_t\|\;\|\sqrt{v^N_\beta}(x_2-x_3)\|
\end{aligned}$$

With Lemma 6.5 it follows that the latter is bounded by the right hand side of (35), thus it suffices to control

$$\widetilde{S}_8:=(N-1)(N-2)\Im\left(\left\langle\Psi,v^N_\beta(x_2-x_3)g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1\Psi\right\rangle\right)$$

and

$$\widetilde{S}_9:=\frac{N!}{(N-3)!}\Im\left(\left\langle\Psi,v^N_\beta(x_1-x_3)g^N_{8/9,1}(x_1-x_2)(\widehat{n}-\widehat{n}_1)p_1\Psi\right\rangle\right)$$

instead of S_8 and S_9. For $\widetilde{S}_8$ we have

$$|\widetilde{S}_8|\quad\leq\quad N^2\|\sqrt{v^N_\beta}(x_2-x_3)\Psi\|\;\|\varphi^{GP}_t\|\;\|g^N_{8/9,1}\|\;\|\sqrt{v^N_\beta}(x_2-x_3)\Psi\|$$

which is again bounded by the right hand side of (35). For $\widetilde{S}_9$

$$|\widetilde{S}_9| \leq N^2\|\sqrt{v_\beta^N}(x_1-x_3)\Psi\|\,\|g_{8/9,1}^N(x_1-x_2)\sqrt{v_\beta^N}(x_1-x_3)p_1\Psi\|\;.$$

Note that due to (23) $\sqrt{v}_{1,3}g_{8/9,1}^N(x_1-x_2)<v_{1,3}a/(N|x_1-x_2|)$ and $g_{8/9,1}^N(x_1-x_2)<C$, thus $\sqrt{v}_{1,3}g_{8/9,1}^N(x_1-x_2)<v_{1,3}\widetilde{g}(x_2-x_3)$ with $\widetilde{g}(x)<C/(N|x|+1)$ and $g(x)=0$ for $x>CN^{-8/9}$. It follows that

$$\|g_{8/9,1}^N(x_1-x_2)\sqrt{v_\beta^N}(x_1-x_3)p_1\Psi\| \leq C\|\varphi_t^{GP}\|_\infty\,\|\sqrt{v_\beta^N}(x_1-x_3)\|\,\|\widetilde{g}(x_2-x_3)\Psi\|$$

Using Hölder and Sobolev it follows that for sufficiently large N

$$\begin{aligned}\|\widetilde{g}(x_2-x_3)\Psi\|^2 &\leq \|\widetilde{g}^2\|_{3/2}\,\|\Psi^2\|_3=\|\widetilde{g}\|_3^2\,\|\Psi\|_6^2\\ &\leq \|\nabla\Psi\|^2\left(\int\widetilde{g}^3d^3x\right)^{2/3}\\ &\leq C\|\nabla\Psi\|^2\left(N^{-3}\int_{N^{-1}<|x|<1}|x|^{-3}d^3x+N^{-3}\right)^{2/3}\\ &\leq CN^{-2}\|\nabla\Psi\|^2(\ln N)^{2/3}\end{aligned}$$

It follows that also $\widetilde{S}_9$ is bounded by the right hand side of (35) and (b) follows.
(c)

□

Similar as for $\alpha_2(\Psi)$ above, we wish to equip $\alpha_1(\Psi)$ with a microscopic structure, i.e. define a $\lambda_1(\Psi)$ and a $\lambda_1'(\Psi)$ such that $\frac{d}{dt}\lambda_1(\Psi)=\lambda_1'(\Psi)$ for any solution of the Schrödinger equation Ψ_t and such that $\alpha_1'(\Psi)-\lambda_1'(\Psi)$ and $\lambda_1(\Psi)$ become controllable for $1/3\leq\beta\leq1$. As a first step we shall define $\lambda_1(\Psi)$ similar as $\lambda_2(\Psi)$ above (c.f. Definition Lemma 6.7) comparing $\alpha_1(\Psi)$ with $\alpha_1(\Psi)$, i.e. we define

$$\lambda_1(\Psi):=N(N-1)\Im\left(\left\langle\Psi,g_{2/7,\beta}^N(x_1-x_2)(\widehat{n}-\widehat{n}_2)p_1p_2\Psi\right\rangle\right)$$

and

$$\begin{aligned}\lambda_1'(\Psi) &:= N(N-1)\Im\left(\left\langle\Psi,\left[H,g_{2/7,\beta}^N(x_1-x_2)(\widehat{n}-\widehat{n}_2)p_1p_2\right]\Psi\right\rangle\right)\\ &\quad -N(N-1)\Im\left(\left\langle\Psi,g_{2/7,\beta}^N(x_1-x_2)\left[H^{GP},(\widehat{n}-\widehat{n}_2)p_1p_2\right]\Psi\right\rangle\right)\;.\end{aligned}$$

As above (Lemma 6.8 (a) and (c)) we have

$$i\frac{d}{dt}\lambda_1(\Psi_t)=\lambda_1'(\Psi_t)\;.$$

Writing

$$\lambda_1(\Psi):=N(N-1)\Im\left(\left\langle(p_1+q_1)\Psi,g_{2/7,\beta}^N(x_1-x_2)(\widehat{n}-\widehat{n}_2)p_1p_2\Psi\right\rangle\right)$$

we get furthermore

$$\begin{aligned}\|\lambda_1(\Psi)\| &\leq CN^2\|\varphi_t^{GP}\|_\infty^2\, \|g^N_{2/7,\beta}\|_1\, N^{-1/2} + CN^2\|\varphi_t^{GP}\|_\infty\, \|g^N_{2/7,\beta}\|\, N^{-1} \\ &\leq C\|\varphi_t^{GP}\|_\infty N^{-1/14}\,.\end{aligned}$$

For $|\lambda_1'(\Psi)-\alpha_1'(\Psi)|$ we can use (36), replacing $g^N_{8/9,\beta}$ by $g^N_{2/7,\beta}$ and $(\widehat{n}-\widehat{n}_1)p_1q_2$ by $(\widehat{n}-\widehat{n}_2)p_1p_2$. Using symmetry, $1=p_j+q_j$ and (17) and reordering the summands we get

$$\begin{aligned}
&\lambda_1'(\Psi)-\alpha_1'(\Psi)\\
=\;& N(N-1)\Im\left(\left\langle p_1\Psi, \left[-a_N\sum_{j=1}^N|\varphi_t^{GP}|^2(x_j), g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-\widehat{n}_2)p_1p_2\right]\Psi\right\rangle\right)\\
&+N(N-1)\Im\left(\left\langle q_1\Psi, \left[-a_N\sum_{j=1}^N|\varphi_t^{GP}|^2(x_j), g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-\widehat{n}_2)p_1p_2\right]\Psi\right\rangle\right)\\
&+N(N-1)\Im\left(\left\langle\Psi, W^N_{2/7,\beta}f^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-\widehat{n}_2)p_1p_2\Psi\right\rangle\right)\\
&-2N(N-1)\Im\left(\left\langle\Psi, p_1(\nabla_2 g^N_{2/7,\beta}(x_1-x_2))\nabla_1 p_1p_2(\widehat{n}-\widehat{n}_1)\Psi\right\rangle\right)\\
&-2N(N-1)\Im\left(\left\langle\Psi, q_1(\nabla_2 g^N_{2/7,\beta}(x_1-x_2))\nabla_1 p_1p_2(\widehat{n}-\widehat{n}_1)\Psi\right\rangle\right)\\
&-N(N-1)\Im\left(\left\langle\Psi, g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-\widehat{n}_2)p_1p_2v^N_\beta(x_1-x_2)\Psi\right\rangle\right)\\
&-2\frac{N!}{(N-3)!}\Im\left(\left\langle\Psi, p_1g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-\widehat{n}_2)p_1p_2v^N_\beta(x_2-x_3)\Psi\right\rangle\right)\\
&-2\frac{N!}{(N-3)!}\Im\left(\left\langle\Psi, q_1g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-\widehat{n}_2)p_1p_2v^N_\beta(x_2-x_3)\Psi\right\rangle\right)\\
&+2\frac{N!}{(N-3)!}\Im\left(\left\langle\Psi, p_1v^N_\beta(x_2-x_3)g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-\widehat{n}_2)p_1p_2\Psi\right\rangle\right)\\
&+2\frac{N!}{(N-3)!}\Im\left(\left\langle\Psi, q_1v^N_\beta(x_2-x_3)g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-\widehat{n}_2)p_1p_2\Psi\right\rangle\right)\\
&+2\frac{N!}{(N-4)!}\Im\left(\left\langle\Psi, v^N_\beta(x_3-x_4)g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-\widehat{n}_1-\widehat{n}_2+\widehat{n}_3)p_1p_2p_3q_3\Psi\right\rangle\right)\\
&-2\frac{N!}{(N-4)!}\Im\left(\left\langle\Psi, g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-\widehat{n}_1-\widehat{n}_2+\widehat{n}_3)p_1p_2p_3q_3v^N_\beta(x_3-x_4)\Psi\right\rangle\right)\\
&+\frac{N!}{(N-4)!}\Im\left(\left\langle\Psi, v^N_\beta(x_3-x_4)g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-2\widehat{n}_2+\widehat{n}_4)p_1p_2p_3p_4\Psi\right\rangle\right)\\
&-\frac{N!}{(N-4)!}\Im\left(\left\langle\Psi, g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-2\widehat{n}_2+\widehat{n}_4)p_1p_2p_3p_4v^N_\beta(x_3-x_4)\Psi\right\rangle\right)\\
=:\;& \sum_{j=0}^{13}T_j\,. \qquad (37)
\end{aligned}$$

For T_0 to T_{11} one can copy the estimates of S_0 to S_{10} above and gets, that

$\sum_{j=0}^{11} T_j$ is bounded by

$$C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)\left(N^{-\gamma} + (\ln N)^{1/3}\alpha(\Psi)\right) . \tag{38}$$

Instead of controlling T_{12} and T_{13} we add another term which pays respect to higher orders of for the microscopic structure, i.e. we define

$$\begin{aligned}\lambda_3(\Psi) \quad := \quad & \frac{N!}{(N-4)!}\Im\left(\left\langle\Psi, g^N_{2/7,\beta}(x_3-x_4)g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-2\widehat{n}_2+\widehat{n}_4)p_1p_2p_3p_4\Psi\right\rangle\right)\\ & -\frac{N!}{(N-4)!}\Im\left(\left\langle\Psi, g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-2\widehat{n}_2+\widehat{n}_4)p_1p_2p_3p_4 g^N_{2/7,\beta}(x_3-x_4)\Psi\right\rangle\right)\end{aligned}$$

and the respective $\lambda_3'(\Psi)$, again with $\frac{d}{dt}\lambda_3(\Psi)=\lambda_3'(\Psi)$.

Controlling $\lambda_3'(\Psi)$ we get similar terms as the T_j above, the only difference being an additional operator $N^2 g^N_{2/7,\beta}(x_j-x_k)p_jp_k$ and a higher order derivative of $\widehat{n}$ (interpreting $\widehat{m}-\widehat{m}_1$ as the derivative of $\widehat{m}$). We arrive at terms which are bounded by (38) and the respective T_{12} and T_{13}, i.e.

$$\frac{N!}{(N-6)!}\Im\left(\left\langle\Psi, V_{5,6}g^N_{2/7,\beta}(x_1-x_2)g^N_{2/7,\beta}(x_3-x_4)(\widehat{n}-3\widehat{n}_2+3\widehat{n}_4-\widehat{n}_6)p_1p_2p_3p_4p_5p_6\Psi\right\rangle\right) ,$$

$$\frac{N!}{(N-6)!}\Im\left(\left\langle\Psi, g^N_{2/7,\beta}(x_1-x_2)g^N_{2/7,\beta}(x_3-x_4)(\widehat{n}-3\widehat{n}_2+3\widehat{n}_4-\widehat{n}_6)p_1p_2p_3p_4p_5p_6V_{5,6}\Psi\right\rangle\right)$$

and

$$\frac{N!}{(N-6)!}\Im\left(\left\langle\Psi, V_{5,6}g^N_{2/7,\beta}(x_1-x_2)(\widehat{n}-3\widehat{n}_2+3\widehat{n}_4-\widehat{n}_6)p_1p_2p_3p_4p_5p_6 g^N_{2/7,\beta}(x_3-x_4)\Psi\right\rangle\right) .$$

Iteratively we add higher orders of the microscopic structure for the remaining terms. Each iteration yields another operator $N^2 g^N_{2/7,\beta}(x_j-x_k)p_jp_k$ and a "higher order derivative of $\widehat{n}$", thus a factor $N^{-1/7}$. We stop the iteration as soon as all the remaining terms can be estimated by (38). Thus we get

Lemma 6.9 *There exists a $\gamma>0$ and functionals $\lambda_1(\Psi)$ and $\lambda_1'(\Psi)$ such that*

(a) For any solution of the Schödinger equation $\Psi_t \in L^2(\mathbb{R}^{3N}\to\mathbb{C})$

$$i\frac{d}{dt}\lambda_1(\Psi_t) = \lambda_1'(\Psi_t)$$

(b) There exist a $C<\infty$ such that for any $\Psi\in L^2(\mathbb{R}^{3N}\to\mathbb{C})$

$$|\lambda_1'(\Psi)-\alpha_1'(\Psi)| \le C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)\left(N^{-\gamma}+(\ln N)^{1/3}\alpha(\Psi)\right) .$$

(c)

$$\|\lambda_1(\Psi)\| \le CN^{-\gamma}\|\varphi_t^{GP}\|_\infty .$$

Summarizing (21) , Lemma 6.8 and Lemma 6.9 and setting $\lambda(\Psi) := \alpha(\Psi) + \lambda_1(\Psi) + \lambda_2(\Psi)$ we arrive at

Corollary 6.10 *There exists a $\gamma > 0$ and functionals $\lambda(\Psi)$ and $\lambda'(\Psi)$ such that*

(a) For any solution of the Schödinger equation $\Psi_t \in L^2(\mathbb{R}^{3N} \to \mathbb{C})$

$$i\frac{d}{dt}\lambda(\Psi_t) = \lambda'(\Psi_t)$$

(b) There exist a $C < \infty$ such that for any $\Psi \in L^2(\mathbb{R}^{3N} \to \mathbb{C})$

$$|\lambda'(\Psi)| \leq C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)\left(N^{-\gamma} + (\ln N)^{1/3}\lambda(\Psi)\right) \ .$$

(c)

$$\|\lambda(\Psi) - \alpha(\Psi)\| \leq CN^{-\gamma}\|\varphi_t^{GP}\|_\infty \ .$$

6.4 Proof of Theorem 4.3 for $\beta \geq 1/3$

In view of Corollary 6.10 (c) and Lemma 2.4 (b) it suffices to prove that

$$\lim_{N\to\infty} \lambda(\Psi_t) = 0$$

under the assumption $\lim_{N\to\infty} N^\gamma\lambda(\Psi_0) = 0$. Therefore we use the estimates we get from Corollary 6.10 (b) on the time derivative of $\lambda(\Psi_t)$ and a Gronwall-like argument.

Using that

$$|\frac{d}{dt}\lambda(\Psi_t)| \leq C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)\left(N^{-\gamma} + (\ln N)^{1/3}\lambda(\Psi_t)\right)$$

it follows that $\lambda(\Psi_t)$ is bounded from above by the solution μ_t of the differential equation

$$\frac{d}{dt}\mu_t = C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)\left(N^{-\gamma} + (\ln N)^{1/3}\mu_t\right) \tag{39}$$

with $\mu_0 = \lambda(\Psi_0)$.

Defining $\zeta_t := N^{-\gamma} + (\ln N)^{1/3}\mu_t$ we get from (39)

$$(\ln N)^{-1/3}\frac{d}{dt}\zeta_t = C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)\zeta_t \ .$$

Thus

$$\zeta_t := K\exp\left(C(\ln N)^{1/3}\int_0^t(\|\varphi_s^{GP}\|_\infty + \|\nabla\varphi_s^{GP}\|_\infty)ds\right)$$

with

$$K = \zeta_0 = N^{-\gamma} + (\ln N)^{1/3}\mu_0 = N^{-\gamma} + (\ln N)^{1/3}\lambda(\Psi_0) < N^{-\gamma}(1 + (\ln N)^{1/3})$$

for N large enough.

Note, that under the assumptions of the Theorem $\int_0^t (\|\varphi_s^{GP}\|_\infty + \|\nabla\varphi_s^{GP}\|_\infty) ds$ is bounded. Note also, that $e^{C(\ln N)^{1/3}} = e^{C(\ln N)(\ln N)^{-2/3}} = N^{C(\ln N)^{-2/3}}$. Since $\lim_{N\to\infty}(\ln N)^{-2/3} = 0$ it follows that $\lim_{N\to\infty} N^{-\gamma} e^{C(\ln N)^{1/3}} = 0$ for any $\gamma > 0$.

Thus ζ_t tends to zero as $N \to \infty$ uniform in $t < T$, so does μ_t and so does $\lambda(\Psi_t)$. With Corollary 6.10 (c) the Theorem follows.

Acknowledgments

Helpful discussions with Detlef Dürr, Jakob Yngvason and Jean-Bernard Bru are gratefully acknowledged.

7 Appendix

It is left to prove the Lemma 5.2, Lemma 5.3 and Lemma 6.6. Since $\|\varphi_t^{GP}\|_\infty$ is bounded we have that for any $m : \{1, \ldots, N\} \to \mathbb{R}^+$ with $m \leq n^{-1}$

$$|\langle\Psi, q_1 p_2 |\varphi_t^{GP}|^2 \widehat{m} q_1 q_2 \Psi\rangle| \leq C\|q_1 p_2 \Psi\| \, \|\widehat{m} q_1 q_2 \Psi\| < C\alpha(\Psi) \; .$$

Note also that $p_j f(x_k) q_j = 0$ for any $k \neq j$ and any function f. So Lemma 5.2, Lemma 5.3 and Lemma 6.6 follow once we have

Lemma 7.1 *Let $m : \{1, \ldots, N\} \to \mathbb{R}^+$ with $m \leq n^{-1}$, $0 < \beta < 1$. Then we have under the conditions of the Theorem that there exists a $C < \infty$ and a $\xi > 0$ such that for any $m : \{1, \ldots, N\} \to \mathbb{R}^+$ with $m \leq \sqrt{n}$*

(a) for any $0 < \beta < 1$

$$|\langle\Psi, p_1 p_2 \left((N-1) v_\beta^N(x_1, x_2) - a|\varphi_t^{GP}|^2(x_1)\right) p_1 p_2 \Psi\rangle| \tag{40}$$
$$\leq C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty) N^{-\xi}$$

$$|\langle\Psi, p_1 p_2 \left((N-1) v_\beta^N(x_1, x_2) - a|\varphi_t^{GP}|^2(x_1)\right) \widehat{m} q_1 p_2 \Psi\rangle| \tag{41}$$
$$\leq C(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty) N^{-\xi}$$

$$|\langle\Psi, p_1 p_2 v_\beta^N(x_1, x_2) q_1 q_2 \Psi\rangle| \tag{42}$$
$$\leq C N^{-1}(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)(\alpha(\Psi) + N^{-\xi})$$

$$|\langle\Psi, q_1 p_2 v_\beta^N(x_1, x_2) \widehat{m} q_1 q_2 \Psi\rangle| \tag{43}$$
$$\leq C N^{-1}(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)(\alpha(\Psi) + N^{-\xi} + \|\mathbb{1}_{\mathcal{S}_1} \nabla_1 q_1 \Psi\|^2)$$

(b) for any $0 < \beta < 1/3$

$$|\langle\Psi, p_1 p_2 v_\beta^N(x_1, x_2) \widehat{m} q_1 q_2 \Psi\rangle| \tag{44}$$
$$\leq C N^{-1}(\|\varphi_t^{GP}\|_\infty + \|\nabla\varphi_t^{GP}\|_\infty)(\alpha(\Psi) + N^{-\xi})$$

Proof:
The right hand side of (40) is bounded by

$$\begin{aligned} S_1 &:= \sup_{x_1\in\mathbb{R}^3}\left\{\left|\left\langle\varphi_t^{GP}(x_2),\left((N-1)v_\beta^N(x_1,x_2)-a|\varphi_t^{GP}|^2(x_1)\right)\varphi_t^{GP}(x_2)\right\rangle_2\right|\right\} \\ &\leq \sup_{x_1\in\mathbb{R}^3}\left\{\left|\left\langle\varphi_t^{GP}(x_1),(N-1)v_\beta^N(x_1-x_2)\varphi_t^{GP}(x_1)\right\rangle_2-a|\varphi_t^{GP}(x_1)|^2\right|\right\} \\ &\quad +(N-1)\sup_{|x_1-x_2|<CN^{-\beta}}\{(|\varphi_t^{GP}(x_1))^2-(\varphi_t^{GP}(x_2))^2|\}\|v_\beta^N\|_1\ . \end{aligned}$$

The first term is equal to $((N-1)\|v_\beta^N\|_1-a)\|\varphi_t^{GP}(x_1)\|_\infty^2$ and in view of Definition 4.2 bounded by $C\|\varphi_t^{GP}\|_\infty^2N^{-\delta}$. Using Taylors formula the second term is of order $\|\nabla\varphi_t^{GP}\|_\infty N^{-\beta}$, thus

$$|S_1|\leq C(\|\varphi_t^{GP}\|_\infty+\|\nabla\varphi_t^{GP}\|_\infty)(N^{-\beta}+N^{-\delta})\ . \tag{45}$$

Since under our assumptions $\|\varphi_t^{GP}\|_\infty+\|\nabla\varphi_t^{GP}\|_\infty<\infty$ (40) follows.

The left hand side of (41) is bounded by

$$S_1\|p_1p_2\Psi\|\ \|\widehat{m}q_1p_2\Psi\|\leq S_1\|p_1p_2\Psi\|\ \|\widehat{n}q_1p_2\Psi\|$$

With (45) and Lemma 2.3 we get (41).

Next we shall prove (44). To estimate this term note, that the operator norm of $p_1p_2v_\beta^N(x_1,x_2)\widehat{m}q_1q_2$ restricted to subspace of symmetric functions is much smaller than the operator norm on full $L^2(\mathbb{R}^{3N}\to\mathbb{C})$. Therefore one has to use symmetry of Ψ to get good control of this term. We define for some $\delta>0$ we shall specify below the functions $m^{a,b}:\{1,\ldots,N\}\to\mathbb{R}^+$ by $m^a(k):=m(k)$ for $k<N^{1-\delta}$, $m^a(k)=0$ for $k\geq N^{1-\delta}$ and $m^b=m-m^a$. It follows that (44) is bounded by

$$|\langle\Psi,p_1p_2v_\beta^N(x_1,x_2)\widehat{m}^aq_1q_2\Psi\rangle|+|\langle\Psi,p_1p_2v_\beta^N(x_1,x_2)\widehat{m}^bq_1q_2\Psi\rangle|_2\Psi\rangle|\ .$$

Defining also $g:\{1,\ldots,N\}\to\mathbb{R}^+$ by $g(k)=1$ for $k<N^{1-\delta}$, $g(k)=0$ for $k\geq N^{1-\delta}$ we have that $m^a=m^as$ and thus

$$\begin{aligned} &\langle\Psi,\widehat{g}_{-2}p_1p_2v_\beta^N(x_1,x_2)q_1q_2\widehat{m}^a\Psi\rangle \\ =\ &(N-1)^{-1}\langle\Psi,\sum_{j=2}^N\widehat{g}_{-2}p_1p_jv_\beta^N(x_1,x_j)q_1q_j\widehat{m}^a\Psi\rangle \\ \leq\ &(N-1)^{-1}\|\sum_{j=2}^N\widehat{g}_{-2}q_jv_\beta^N(x_1,x_j)p_1p_j\Psi\|\ \|\widehat{m}^aq_1\Psi\|\ . \end{aligned} \tag{46}$$

Using Lemma 2.3 (d)

$$\begin{aligned}
& \langle\Psi, p_1 p_2 v_\beta^N(x_1,x_2) q_1 q_2 \widehat{m}^b \Psi\rangle \\
= \quad & (N-1)^{-1}\langle\Psi, \sum_{j=2}^N (\widehat{m}^b_{-2})^{1/2} p_1 p_j v_\beta^N(x_1,x_j) q_1 q_j (\widehat{m}^b)^{1/2}\Psi\rangle \\
\leq \quad & (N-1)^{-1}\| \sum_{j=2}^N q_j v_\beta^N(x_1,x_j) p_1 p_j \Psi\| \, \|(\widehat{m}^b)^{1/2} q_1 \Psi\| \\
\leq \quad & (N-1)^{-1}\| \sum_{j=2}^N q_j v_\beta^N(x_1,x_j) p_1 p_j \Psi\| \; \alpha(\Psi) \; . \qquad (47)
\end{aligned}$$

For any $h : \{1,\dots,N\} \to \mathbb{R}^+$ we have that

$$\begin{aligned}
& \| \sum_{j=2}^N \widehat{h} q_j v_\beta^N(x_1,x_j) p_1 p_j \Psi\|^2 \\
= \quad & \sum_{j\neq k\neq 1} \langle \widehat{h}\Psi, p_1 q_k \sqrt{v_\beta^N}(x_1,x_k) p_j \sqrt{v_\beta^N}(x_1,x_j) \\
& \qquad \sqrt{v_\beta^N}(x_1,x_k) p_k \sqrt{v_\beta^N}(x_1,x_j) p_1 q_j \widehat{h}\Psi\rangle \\
& + \sum_{j=2}^N \langle \widehat{h}\Psi, p_1 p_j v_N(x_1,x_j) q_j v_N(x_1,x_j) p_1 p_j \widehat{h}\Psi\rangle \\
\leq \quad & (N-1)(N-2)\|\sqrt{v}_N(x_1,x_2)p_2\|_{op}^4 \; \|q_3 \widehat{h}\Psi\|^2 \\
& + C N^{1/2}(N-1)\|(v_\beta^N)^2\|_1 \|\varphi_t^{GP}\|_\infty^2 \|\widehat{h}\|^2 \\
\leq \quad & C(N-1)(N-2)N^{-2}\|\varphi_t^{GP}\|_\infty^4 \|\widehat{h}\widehat{n}\Psi\|^2 \\
& + C(N-1)N^{1/2}N^{-2+3\beta}\|\varphi_t^{GP}\|_\infty^2 \sup_{1\leq k\leq N}|h(k)^2|
\end{aligned}$$

where we used Lemma 2.3 as well as that under our conditions $\|v_\beta^N\|_\infty \leq CN^{3\beta}$.

Note that $\sup_{1\leq k\leq N}|g(k)^2| = 1$ and $\sup_{1\leq k\leq N}|m^b(k)| = N^\delta$. Note also that $\|\widehat{m}^b_{-2}\widehat{n}\Psi\|^2 \leq \|\widehat{n}^{1/2}_{-2}\Psi\|^2 \leq \alpha(\Psi) + 2N^{-1/2}$ and $s(k-2)n(k) < CN^{-\delta}$. Thus

$$|\langle\Psi, p_1 p_2 v_\beta^N(x_1,x_2)\widehat{m} q_1 q_2\Psi\rangle| \leq CN^{-1}\|\varphi_t^{GP}\|_\infty^2 \left(\alpha(\Psi) + N^{-1+3\beta+2\delta} + N^{-\delta}\right) \; .$$

Choosing $0 < \delta < (-1+3\beta)/2$ and $\xi < \min\{-1+3\beta+2\delta, \delta\}$ (44) follows.

(42) for $0 \leq \beta < 1/3$ can be proven in the same way replacing $\widehat{m}$ by 1. For $1/3 \leq \beta < 1$ we define

$$U_N(\mathbf{x}) := \begin{cases} \frac{3}{4\pi}\|v_\beta^N\|_1 N^{3/4}, & \text{for } x < N^{-1/4}; \\ 0, & \text{else.} \end{cases}$$

and

$$h_N(x) := \int |x-y|^{-1}(v_\beta^N(y) - U_N(y))d^3y \qquad (48)$$

By this Definition it follows that $h_N(x) = 0$ for $x > N^{-1/4}$, $|h_N| < \|v_\beta^N\|_1 |x|^{-1}$, $|\nabla h_N| < \|v_\beta^N\|_1 |x|^{-2}$, thus

$$\|h_N\|_\infty < CN^{-1+3\beta} \qquad \|h_N\| < CN^{-1-\beta/2} \tag{49}$$

and

$$-\Delta h_N = v_\beta^N - U_N \ .$$

So having proven (42) for $\beta < 1/3$, (42) follows once we have

$$|\langle \Psi, p_1 p_2 (\Delta h_N)(x_1 - x_2) q_1 q_2 \Psi\rangle| \leq C(\|\varphi_t^{GP}\|_\infty + \|\nabla \varphi_t^{GP}\|_\infty) N^{-\xi} \ . \tag{50}$$

Integration by parts and Lemma 2.3 (d) yield

$$\begin{aligned} |\langle \Psi, p_1 p_2 (\Delta h_N) q_1 q_2 \Psi\rangle| \quad &\leq \quad |\langle \Psi, p_1 p_2 (\nabla_1 h_N(x_1 - x_2)) \nabla_1 q_1 q_2 \Psi\rangle| \\ &\quad\quad + |\langle \nabla_1 p_1 p_2 \Psi, (\nabla_1 h_N(x_1 - x_2)) q_1 q_2 \Psi\rangle| \\ &=: \quad S_2 + S_3 \ . \end{aligned}$$

For S_2 we have similar as above

$$\begin{aligned} & |\langle \Psi, p_1 p_2 (\nabla_1 h_N(x_1 - x_2)) \nabla_1 q_1 q_2 \Psi\rangle| && (51) \\ = \quad & (N-1)^{-1} |\sum_{j=2}^N \langle \Psi, p_1 p_j (\nabla_1 h_N(x_1 - x_j)) \nabla_1 q_1 q_j \Psi\rangle| && (52) \\ \leq \quad & (N-1)^{-1} \|\nabla_1 q_1 \Psi\| \, \|\sum_{j=2}^N q_j (\nabla_1 h_N(x_1 - x_j)) p_1 p_j \Psi\| && (53) \end{aligned}$$

For the last factor we write

$$\begin{aligned} & \|\sum_{j=2}^N q_j (\nabla_1 h_N(x_1 - x_j)) p_1 p_j \Psi\| \\ = \quad & \sum_{j \neq k \neq 1} \langle \Psi, p_1 p_k (\nabla_1 h_N(x_1 - x_j)) q_k q_j (\nabla_1 h_N(x_1 - x_k)) p_1 p_j \Psi\rangle \\ & + \sum_{j=2}^N \langle \Psi, p_1 p_j (\nabla_1 h_N(x_1 - x_j))^2 p_1 p_j \Psi\rangle \\ =: \quad & S_4 + S_5 \ . \end{aligned}$$

Note, that $\nabla_1 h_N(x_1 - x_2) = -\nabla_2 h_N(x_1 - x_2)$, thus

$$S_4 \quad = \quad \sum_{j \neq k \neq 1} \langle \Psi, p_1 p_k q_j (\nabla_j h_N(x_1 - x_j))(\nabla_k h_N(x_1 - x_k)) p_1 p_j q_k \Psi\rangle$$

Partial integrations yield

$$
\begin{aligned}
S_4 &= \sum_{j\neq k\neq 1} \langle \nabla_j \nabla_k p_1 p_k q_j \Psi, h_N(x_1-x_j) h_N(x_1-x_k) p_1 p_j q_k \Psi\rangle \\
&\quad + \sum_{j\neq k\neq 1} \langle \nabla_j p_1 p_k q_j \Psi, h_N(x_1-x_j) h_N(x_1-x_k) \nabla_k p_1 p_j q_k \Psi\rangle \\
&\quad + \sum_{j\neq k\neq 1} \langle \nabla_k p_1 p_k q_j \Psi, h_N(x_1-x_j) h_N(x_1-x_k) p_1 \nabla_j p_j q_k \Psi\rangle \\
&\quad + \sum_{j\neq k\neq 1} \langle p_1 p_k q_j \Psi, h_N(x_1-x_j) h_N(x_1-x_k) \nabla_j \nabla_k p_1 p_j q_k \Psi\rangle \ ,
\end{aligned}
$$

so as above S_4 is bounded by the right hand side of (42). For S_5 we estimate

$$
\|(\nabla_1 h_N(x_1-x_j))^2\|_1 = h_N(x_1-x_j)\Delta_1 h_N(x_1-x_j)
$$

which is (see below (48)) of order $N^{-2+3\beta}$. Thus S_2 is bounded by the right hand side of (42).

For S_3 note, that $\nabla_1 h_N(x_1-x_2) = -\nabla_2 h_N(x_1-x_2)$. Integration by parts yields

$$
\begin{aligned}
S_3 &\leq |\langle \nabla_1\nabla_2 p_1 p_2 \Psi, h_N(x_1-x_2) q_1 q_2 \Psi\rangle| \\
&\quad + |\langle \nabla_1 p_1 p_2 \Psi, h_N(x_1-x_2) \nabla_2 q_1 q_2 \Psi\rangle| \\
&\leq \|\nabla\varphi_t^{GP}\|_\infty^2 \ \|h_N^2(x_1-x_2)\|_1^{1/2} \ \|q_1 q_2 \Psi\| \\
&\quad + \|\nabla\varphi_t^{GP}\|_\infty \ \|\varphi_t^{GP}\|_\infty \ \|h_N^2(x_1-x_2)\|_1^{1/2} \ \|\nabla_2 q_1 q_2 \Psi\|
\end{aligned}
$$

and (50) and thus (42) follows.

Next we shall prove (43). We define

$$
h_N(x) := \int |x-y|^{-1} v_\beta^N(y) d^3y \ . \tag{54}
$$

As above this definition implies that $|h_N| < \|v_\beta^N\|_1 |x|^{-1}$, $|\nabla h_N| < \|v_\beta^N\|_1 |x|^{-2}$, $\|h_N\|_\infty < CN^{-1+3\beta}$, $\|h_N\| < CN^{-1-\beta/2}$ and

$$
-\Delta h_N = v_\beta^N \ .
$$

$$
\begin{aligned}
|\langle \Psi, q_1 p_2 v_\beta^N(x_1-x_2) \widehat{m} q_1 q_2 \Psi\rangle| &= |\langle \Psi, \widehat{m}_2 q_1 p_2 (\Delta h_N)(x_1-x_2) q_1 q_2 \Psi\rangle| \\
&= \langle \Psi, q_1 p_2 \widehat{m}_2 (\Delta h_N) q_1 q_2 \Psi\rangle| \\
&\leq |\langle \Psi, q_1 p_2 \widehat{m}_2 (\nabla_1 h_N(x_1-x_2)) \mathbb{1}_{\mathcal{S}_1} \nabla_1 q_1 q_2 \Psi\rangle| \\
&\quad + |\langle \Psi, q_1 p_2 \widehat{m}_2 (\nabla_1 h_N(x_1-x_2)) \mathbb{1}_{\overline{\mathcal{S}}_1} \nabla_1 q_1 q_2 \Psi\rangle| \\
&\quad + |\langle \nabla_1 q_1 p_2 \widehat{m}_2 \Psi, (\nabla_1 h_N(x_1-x_2)) q_1 q_2 \Psi\rangle| \\
&=: S_6 + S_7 + S_8 \ .
\end{aligned}
$$

For S_6 we have

$$\begin{aligned} S_6 &= (N-1)^{-1}|\sum_{j=2}^{N}\langle\Psi, q_1p_j\widehat{m}_2(\nabla_1 h_N(x_1-x_j))\mathbb{1}_{\mathcal{S}_1}\nabla_1 q_1q_j\Psi\rangle| \\ &\leq (N-1)^{-1}\|\mathbb{1}_{\mathcal{S}_1}\nabla_1 q_1\Psi\|\,\|\sum_{j=2}^{N}q_j(\nabla_1 h_N(x_1-x_j))\widehat{m}_2 q_1p_j\Psi\|\,. \end{aligned}$$

For the last factor we write

$$\begin{aligned} &\|\sum_{j=2}^{N}q_j(\nabla_1 h_N(x_1-x_j))\widehat{m}_2 q_1p_j\Psi\|^2 \\ =\;& \sum_{j\neq k\neq 1}\langle\Psi, \widehat{m}_2 q_1p_k(\nabla_1 h_N(x_1-x_j))q_kq_j(\nabla_1 h_N(x_1-x_j))\widehat{m}_2 q_1p_j\Psi\rangle \\ &+\sum_{j=2}^{N}\langle\Psi, \widehat{m}_2q_1p_j(\nabla_1 h_N(x_1-x_j))^2\widehat{m}_2q_1p_j\Psi\rangle \\ =:\;& S_9+S_{10}\,. \end{aligned}$$

Note, that $\nabla_1 h_N(x_1-x_2)=-\nabla_2 h_N(x_1-x_2)$, thus

$$S_9 = \sum_{j\neq k\neq 1}\langle\Psi, \widehat{m}_2q_1p_kq_j(\nabla_j h_N(x_1-x_j))(\nabla_k h_N(x_1-x_k))\widehat{m}_2q_1p_jq_k\Psi\rangle$$

Partial integrations yield

$$\begin{aligned} S_9 &= \sum_{j\neq k\neq 1}\langle\nabla_j\nabla_k\widehat{m}_2q_1p_kq_j\Psi, h_N(x_1-x_j)h_N(x_1-x_k)\widehat{m}_2q_1p_jq_k\Psi\rangle \\ &\quad+\sum_{j\neq k\neq 1}\langle\nabla_j\widehat{m}_2q_1p_kq_j\Psi, h_N(x_1-x_j)h_N(x_1-x_k)\nabla_k\widehat{m}_2q_1p_jq_k\Psi\rangle \\ &\quad+\sum_{j\neq k\neq 1}\langle\nabla_k\widehat{m}_2q_1p_kq_j\Psi, h_N(x_1-x_j)h_N(x_1-x_k)\widehat{m}_2q_1\nabla_jp_jq_k\Psi\rangle \\ &\quad+\sum_{j\neq k\neq 1}\langle\widehat{m}_2q_1p_kq_j\Psi, h_N(x_1-x_j)h_N(x_1-x_k)\nabla_j\nabla_k\widehat{m}_2q_1p_jq_k\Psi\rangle\,, \end{aligned}$$

Using symmetry of Ψ

$$\begin{aligned} |S_9| \leq\;& 2(N-1)(N-2)|\langle\mathbb{1}_{\mathcal{S}_2}\nabla_2\nabla_3\widehat{m}_2q_1p_3q_2\Psi, h_N(x_1-x_2)h_N(x_1-x_3)\widehat{m}_2q_1p_2q_3\Psi\rangle| \\ &+2(N-1)(N-2)|\langle\mathbb{1}_{\mathcal{S}_2}\nabla_2\widehat{m}_2q_1p_3q_2\Psi, h_N(x_1-x_2)h_N(x_1-x_3)\mathbb{1}_{\mathcal{S}_3}\nabla_3\widehat{m}_2q_1p_2q_3\Psi\rangle| \\ &+2(N-1)(N-2)|\langle\mathbb{1}_{\overline{\mathcal{S}}_2}\nabla_2\nabla_3\widehat{m}_2q_1p_3q_2\Psi, h_N(x_1-x_2)h_N(x_1-x_3)\widehat{m}_2q_1p_2q_3\Psi\rangle| \\ &+2(N-1)(N-2)|\langle\mathbb{1}_{\overline{\mathcal{S}}_2}\nabla_2\widehat{m}_2q_1p_3q_2\Psi, h_N(x_1-x_2)h_N(x_1-x_3)\mathbb{1}_{\mathcal{S}_3}\nabla_3\widehat{m}_2q_1p_2q_3\Psi\rangle| \\ &+2(N-1)(N-2)|\langle\mathbb{1}_{\overline{\mathcal{S}}_2}\nabla_2\widehat{m}_2q_1p_3q_2\Psi, h_N(x_1-x_2)h_N(x_1-x_3)\mathbb{1}_{\overline{\mathcal{S}}_3}\nabla_3\widehat{m}_2q_1p_2q_3\Psi\rangle|\,, \end{aligned}$$

so as above S_9 is bounded by the right hand side of (42). For S_{10} we estimate

$$\|(\nabla_1 h_N(x_1-x_j))^2\|_1 = h_N(x_1-x_j)\Delta_1 h_N(x_1-x_j)$$

which is (see below (48)) of order $N^{-2+3\beta}$. Using $|ab| < a^2 + b^2$ we get that S_6 is bounded by the right hand side of (43).

For S_7 we have using symmetry

$$\begin{aligned} S_7 &= \frac{1}{N-1}\Big|\sum_{j=2}^{N}\langle\Psi, q_1 p_j \widehat{m}_2(\nabla_1 h_N(x_1-x_j))\mathbb{1}_{\overline{\mathcal{S}}_1}\nabla_1 q_1 q_j\Psi\rangle\Big| \\ &\leq \frac{1}{N-1}\Big\|\sum_{j=2}^{N} q_j(\nabla_1 h_N(x_1-x_j))q_1 p_j \widehat{m}_2\Psi\Big\|\;\|\mathbb{1}_{\overline{\mathcal{S}}_1}\nabla_1 q_1\Psi\|\,. \end{aligned} \tag{55}$$

Using again symmetry we have

$$\begin{aligned} &\Big\|\sum_{j=2}^{N} q_j(\nabla_1 h_N(x_1-x_j))q_1 p_j \widehat{m}_2\Psi\Big\|^2 \\ \leq\; &\sum_{j=2}^{N}\|q_j(\nabla_1 h_N(x_1-x_j))q_1 p_j\widehat{m}_2\Psi\|^2 \\ &+\sum_{j\neq k\neq 1}\langle\Psi, \widehat{m}_2 q_1 p_k h_N(x_1-x_k))q_k q_j(\nabla_1 h_N(x_1-x_j))q_1 p_j \widehat{m}_2\Psi\rangle \\ =\; &(N-1)\|q_j(\nabla_1 h_N(x_1-x_2))q_1 p_2\widehat{m}_2\Psi\|^2 \\ &+(N-1)(N-2)\langle\Psi, \widehat{m}_2 q_1 q_3 p_2(\nabla_1 h_N(x_1-x_2))(\nabla_1 h_N(x_1-x_3))q_1 q_2 p_3\widehat{m}_2\Psi\rangle \end{aligned} \tag{56}$$

For the first summand we have

$$\begin{aligned} (N-1)\|q_j(\nabla_1 h_N(x_1-x_2))q_1 p_2\widehat{m}_2\Psi\|^2 &\leq (N-1)\|(\nabla_1 h_N(x_1-x_2))\|^2\,\|\varphi_t^{GP}\|_\infty^2\,\|\widehat{m}_2 q_1 p_2\Psi\| \\ &\leq C(N-1)\|\varphi_t^{GP}\|_\infty^2\,N^{-2}N^{\beta}\leq CN^{\beta-1} \end{aligned} \tag{57}$$

For the second summand of the right hand side of (56) we get using $\nabla_1 h_N(x_1 - x_2) = -\nabla_2 h_N(x_1-x_2)$, integrating by parts and using symmetry

$$\begin{aligned} &(N-1)(N-2)\langle\Psi, \widehat{m}_2 q_1 q_3 p_2(\nabla_2 h_N(x_1-x_2))(\nabla_3 h_N(x_1-x_3))q_1 q_2 p_3\widehat{m}_2\Psi\rangle \\ =\; &2(N-1)(N-2)\langle\mathbb{1}_{\mathcal{S}_3}\nabla_3 q_1 q_3\nabla_2 p_2\widehat{m}_2\Psi, (h_N(x_1-x_2))(h_N(x_1-x_3))q_1 q_2 p_3\widehat{m}_2\Psi\rangle \\ &+2(N-1)(N-2)\langle\nabla_3 q_1 q_3\nabla_2 p_2\widehat{m}_2\Psi, (h_N(x_1-x_2))(h_N(x_1-x_3))\mathbb{1}_{\overline{\mathcal{S}}_3} q_1 q_2 p_3\widehat{m}_2\Psi\rangle \\ &+(N-1)(N-2)\langle q_1 q_3\nabla_2 p_2\widehat{m}_2\Psi, (h_N(x_1-x_2))(h_N(x_1-x_3))q_1 q_2\nabla_3 p_3\widehat{m}_2\Psi\rangle \\ &+(N-1)(N-2)\langle\mathbb{1}_{\mathcal{S}_3}\nabla_3 q_1 q_3 p_2\widehat{m}_2\Psi, (h_N(x_1-x_2))(h_N(x_1-x_3))q_1\mathbb{1}_{\mathcal{S}_2}\nabla_2 q_2 p_3\widehat{m}_2\Psi\rangle \\ &+(N-1)(N-2)\langle\mathbb{1}_{\mathcal{S}_3}\mathbb{1}_{\overline{\mathcal{S}}_2}\nabla_3 q_1 q_3 p_2\widehat{m}_2\Psi, (h_N(x_1-x_2))(h_N(x_1-x_3))q_1\nabla_2 q_2 p_3\widehat{m}_2\Psi\rangle \\ &+(N-1)(N-2)\langle\nabla_3 q_1 q_3 p_2\widehat{m}_2\Psi, (h_N(x_1-x_2))(h_N(x_1-x_3))\mathbb{1}_{\overline{\mathcal{S}}_3} q_1\nabla_2 q_2 p_3\widehat{m}_2\Psi\rangle \\ \leq\; &2CN^2\|\mathbb{1}_{\mathcal{S}_3}\nabla_3 q_1 q_3\widehat{m}_2\Psi\|\,\|\nabla\varphi_t^{GP}\|_\infty\,\|h_N\|^2\,\|\varphi_t^{GP}\|_\infty\,\|q_1 q_2\widehat{m}_2\Psi\| \\ &+2N^2\|\nabla_3 q_1 q_3\widehat{m}_2\Psi\|\,\|\nabla\varphi_t^{GP}\|_\infty\,\|h_N\|\,\|h_N\|_\infty\sqrt{N}\|\mathbb{1}_{s_{1,2}}\|\,\|\varphi_t^{GP}\|_\infty\,\|q_1 q_2\widehat{m}_2\Psi\| \\ &+N^2\|q_1 q_2\widehat{m}_2\Psi\|^2\,\|h_N\|^2\,\|\nabla\varphi_t^{GP}\|_\infty^2 \\ &+N^2\|\mathbb{1}_{\mathcal{S}_2}\nabla_2 q_1 q_2 p_2\widehat{m}_2\Psi\|^2\,\|h_N\|^2\,\|\varphi_t^{GP}\|_\infty^2 \\ &+2N^2\|\mathbb{1}_{\overline{\mathcal{S}}_3}\|\,\|\varphi_t^{GP}\|_\infty\,\|\nabla_3 q_1 q_3\widehat{m}_2\Psi\|\,\|\varphi_t^{GP}\|_\infty^2\,\|h_N\|^2\,\|q_1\nabla_2 q_2 p_3\widehat{m}_2\Psi\|\,. \end{aligned} \tag{58}$$

Since with (34)

$$\|\mathbb{1}_{\overline{\mathcal{S}}_3}\| = \|\mathbb{1}_{\overline{\mathcal{S}}_3}\|_1^{1/2} = \frac{3}{4\pi}N^{-17/9}$$

(58) is bounded by $C(\alpha(\Psi) + N^{-1/18})$. With (55), (56) and (57) and using $|ab| < a^2 + b^2$ it follows that S_7 is bounded by the right hand side of (43).

For S_8 note, that $\nabla_1 h_N(x_1 - x_2) = -\nabla_2 h_N(x_1 - x_2)$. Integration by parts yields

$$\begin{aligned} S_8 \quad &\leq \quad |\langle \nabla_1 \nabla_2 q_1 p_2 \Psi, h_N(x_1 - x_2)\widehat{m}_1 q_1 q_2 \Psi\rangle| \\ &\quad\quad +|\langle \nabla_1 q_1 p_2 \Psi, h_N(x_1 - x_2)\nabla_2 \widehat{m}_1 q_1 q_2 \Psi\rangle| \\ &\leq \quad \|\nabla \varphi_t^{GP}\|_\infty^2 \, \|h_N\| \, \|\widehat{m}_1 q_1 q_2 \Psi\| \\ &\quad\quad +\|\nabla \varphi_t^{GP}\|_\infty \, \|\varphi_t^{GP}\|_\infty \, \|h_N\| \, \|\widehat{m}_1 q_1 \nabla_2 q_2 \Psi\| \end{aligned}$$

which is in view of Lemma 2.3 and (49) of order $N^{-1-\beta/2}$ and (43) follows.

□

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** (2006), no. 12, 16591741.

[2] Erdös, L.; Schlein, B.; Yau, H.-T.: Derivation of the cubic non-linear Schrodinger equation from quantum dynamics of many-body systems. Invent. Math. **167** (2007), 515614.

[3] Erdös, L.; Schlein, B.; Yau, H.-T.: Derivation of the Gross-Pitaevskii Equation for the Dynamics of Bose-Einstein Condensate. Preprint arXiv:math-ph/0606017. To appear in Ann. Math.

[4] Erdös, L.; Schlein, B.; Yau, H.-T.: Rigorous Derivation of the Gross-Pitaevskii Equation with a Large Interaction Potential arXiv:math-ph/0802.3877v2

[5] Lieb, E.H.; Seiringer, R.: Proof of Bose-Einstein condensation for dilute trapped gases. Phys. Rev. Lett. **88** (2002), 170409-1-4.

[6] Lieb, E.H.; Seiringer, R.; Solovej, J.P.; Yngvason, J.: The mathematics of the Bose gas and its condensation. Oberwolfach Seminars, **34** Birkhauser Verlag, Basel, 2005.

[7] Lieb, E.H.; Seiringer, R.; Yngvason, J.: Bosons in a trap: a rigorous derivation of the Gross- Pitaevskii energy functional. Phys. Rev A **61** (2000), 043602.

[8] Fröhlich, J.; Knowles, A. and Pizzo, A.: Atomism and quantization. J. Phys. A: Math. Theor. **40** (2007) 3033-3045