
Derivation of Mean Field Dynamics for Attractive Quantum Systems

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Abstract

This thesis provides a mathematical rigorous derivation of the cubic nonlinear Schrödinger equation for several many-body systems. In particular, we focus on dynamical systems where the interaction potential is either partly or purely attractive.

First, we study the dynamics of a Bose-Einstein condensate in two dimensions. We consider the interaction potential to be given either by $W_\beta(x) = N^{-1+2\beta}W(N^\beta x)$ for any $\beta > 0$, or by $V_N(x) = e^{2N}V(e^N x)$. Both W and V are spherical symmetric and compactly supported potentials, $W, V \in L^\infty(\mathbb{R}^2, \mathbb{R})$ and may have a sufficiently small negative part. In both cases we prove the convergence of the reduced density matrix corresponding to the exact time evolution to the projector onto the solution of the corresponding nonlinear Schrödinger equation in trace norm. For the latter potential V_N we show that it is crucial to take the microscopic structure of the condensate into account in order to obtain the correct dynamics.

Next, we derive the three dimensional time-dependent Gross-Pitaevskii equation starting from an interacting N -particle system of bosons. Our work extends a previous result on nonnegative interaction potentials [60] to more generic interaction potentials which may have a sufficiently small negative part. To this end we use an operator inequality that was first proven by Jun Yin in [72] as one key estimate.

Finally, we present a microscopic derivation of the two-dimensional focusing cubic nonlinear Schrödinger equation. The interaction potential we consider is given by $W_\beta(x) = N^{-1+2\beta}W(N^\beta x)$ for some spherically symmetric and compactly supported potential $W \in L^\infty(\mathbb{R}^2, \mathbb{R})$. The class of initial wave functions is chosen such that the variance in energy is small. Furthermore, we assume that the Hamiltonian $H_{W_\beta, t} = -\sum_{j=1}^N \Delta_j + \sum_{1 \leq j < k \leq N} W_\beta(x_j - x_k) + \sum_{j=1}^N A_t(x_j)$ fulfills stability of second kind, that is $H_{W_\beta, t} \geq -CN$. We then prove the convergence of the reduced density matrix corresponding to the exact time evolution to the projector onto the solution of the corresponding nonlinear Schrödinger equation in either Sobolev trace norm, if $\|A_t\|_p < \infty$ for some $p > 2$, or in trace norm, for more general external potentials. For trapping potentials of the form $A(x) = C|x|^s$, $C > 0$, the condition $H_{W_\beta, t} \geq -CN$ can be fulfilled for a certain class of interactions W_β , for all $0 < \beta < \frac{s+1}{s+2}$, see [47].

The derivations are based on a method developed by Pickl in [Lett. Math. Phys. 97(2), 151–164 (2011)]. This thesis is based on the preprints [25, 26, 27].

Zusammenfassung

Diese Arbeit befasst sich mit mathematisch rigorosen Herleitungen der kubischen nicht-linearen Schrödinger-Gleichung für mehrere Vierteilchensysteme. Wir sind insbesondere an dynamischen Systemen interessiert, deren Wechselwirkungspotential teilweise oder komplett attraktiv gewählt werden kann.

Zunächst untersuchen wir die Dynamik eines Bose-Einstein Kondensates in zwei Dimensionen. Das Wechselwirkungspotential ist hierbei entweder durch $W_\beta(x) = N^{-1+2\beta}W(N^\beta x)$, für alle $\beta > 0$, oder durch $V_N(x) = e^{2N}V(e^N x)$ gegeben. Sowohl V , als auch W werden als sphärisch symmetrisch und mit kompakten Träger angenommen, mit $W, V \in L^\infty(\mathbb{R}^2, \mathbb{R})$. Weiterhin können W und V einen genügend kleinen negativen Anteil besitzen. In beiden Fällen beweisen wir die Konvergenz der reduzierten Dichtematrix der exakten Zeitentwicklung gegen den Projektor auf die Lösung der entsprechenden nichtlinearen Schrödinger-Gleichung. Die Konvergenz ist hierbei in der Spurnorm zu verstehen. Für das Potential V_N zeigen wir, dass es entscheidend ist, die mikroskopische Struktur des Kondensats zu berücksichtigen, um die korrekte Dynamik zu erhalten.

Als nächstes leiten wir die dreidimensionale zeitabhängige Gross-Pitaevskii-Gleichung ausgehend von einem wechselwirkenden N -Teilchen System von Bosonen her. Unsere Arbeit erweitert ein früheres Resultat [60] auf Wechselwirkungspotentiale, die nicht nichtnegativ sein müssen, sondern einen ausreichend kleinen negativen Teil aufweisen können. Eine Schlüsselabschätzung in unserem Beweis ist eine Operatorungleichung, welche zuerst von Jun Yin bewiesen wurde, siehe [72].

Zuletzt präsentieren wir eine mikroskopische Herleitung der zweidimensionalen kubischen nichtlinearen Schrödinger-Gleichung. Das Wechselwirkungspotential, das wir in Betracht ziehen, ist gegeben durch $W_\beta(x) = N^{-1+2\beta}W(N^\beta x)$, wobei $W \in L^\infty(\mathbb{R}^2, \mathbb{R})$ als sphärisch symmetrisch und mit kompakten Träger angenommen wird. Die Klasse der anfänglichen Wellenfunktionen wird so gewählt, dass die Varianz in der Energie klein ist. Außerdem nehmen wir an, dass der Hamilton-Operator $H_{W_\beta, t} = -\sum_{j=1}^N \Delta_j + \sum_{1 \leq j < k \leq N} W_\beta(x_j - x_k) + \sum_{j=1}^N A_t(x_j)$ die Stabilität der zweiten Art erfüllt, d.h. es ist $H_{W_\beta, t} \geq -CN$ gegeben. Wir beweisen die Konvergenz der reduzierten Dichte-Matrix der exakten Zeitentwicklung gegen den Projektor auf die Lösung der entsprechenden nichtlinearen Schrödinger-Gleichung. Diese Konvergenz erfolgt im Falle $\|A_t\|_p < \infty$, für $p > 2$, in der Sobolev-Spurnorm, für allgemeinere externe Potenziale erfolgt diese in der Spurnorm. Für Potentiale der Form $A(x) = C|x|^s$, $C > 0$, kann die Bedingung $H_{W_\beta, t} \geq -CN$ für eine bestimmte Klasse von

Wechselwirkungen W_β erfüllt werden, für alle $0 < \beta < \frac{s+1}{s+2}$, siehe [47].

Die in der Arbeit vorgenommenen Herleitungen basieren auf einer Arbeit von Pickl [Lett. Math. Phys. 97(2), 151–164 (2011)].

Diese Dissertation basiert auf den Vorveröffentlichungen [25, 26, 27].

Chapter 1

Preface

This work is about the rigorous derivation of effective evolution equations from bosonic many-body systems. On a fundamental level, the dynamics of N interacting bosons is described by the time-dependent Schrödinger equation

$$i\partial_t \Psi_t = H \Psi_t, \quad (1.1)$$

where the nonrelativistic Hamiltonian H is given by

$$H = \sum_{k=1}^N (-\Delta_k) + \sum_{i < j=1}^N V^{(N)}(x_i - x_j) + \sum_{k=1}^N A_t(x_k). \quad (1.2)$$

$V^{(N)}$ describes a pair potential which is N -dependent and A_t is a time-dependent external potential. The interaction $V^{(N)}$ can be thought as strong and short ranged and we will argue in detail for appropriate choices for $V^{(N)}$ below. The initial wavefunction is chosen from the bosonic space $\Psi_0 \in L_s^2(\mathbb{R}^{dN}, \mathbb{C})$, $\|\Psi_0\| = 1$, consisting of all $\Psi \in L^2(\mathbb{R}^{dN}, \mathbb{C})$ which are symmetric under pairwise permutations of the variables $x_1, \dots, x_N \in \mathbb{R}^d$. In this thesis, we are considering the spatial dimensions $d = 2, 3$.

While the dynamics of N interacting bosons is given by the Schrödinger equation above, the exact solution of Ψ_t is hard to analyze or even not tractable. For large particle number N and certain physical systems, one may apply a statistical description of the system, however. This procedure is common practice within the physical community and yields to evolution equations which are easier to discuss. Examples of such approximations are numerous and are in many circumstances in agreement with the observed physical properties of e.g. gases, fluids, conductors, plasmas and solids. Heuristically, it is often possible to argue whether an approximation might be applicable. In this thesis, we will justify the validity of several effective theories by providing a mathematical rigorous analysis. We are in particular interested in the description of Bose-Einstein condensates.

The dynamics of (1.1) will be analyzed at the level of reduced density matrices. For this, we define the one particle reduced density matrix $\gamma_\Psi^{(1)}$ of Ψ with integral kernel

$$\gamma_\Psi^{(1)}(x, x') = \int_{\mathbb{R}^{dN-d}} \Psi^*(x, x_2, \dots, x_N) \Psi(x', x_2, \dots, x_N) dx_2 \dots dx_N. \quad (1.3)$$

$\gamma_{\Psi}^{(1)}$ corresponds to the marginal distribution of Ψ , describing the distribution of one-particle observables. To be more precise, let $\mathcal{B}(L^2(\mathbb{R}^d, \mathbb{C}))$ be the set of all bounded operators on the one particle Hilbert space $L^2(\mathbb{R}^d, \mathbb{C})$. Then, for $A \in \mathcal{B}(L^2(\mathbb{R}^d, \mathbb{C}))$

$$\text{tr}(\gamma_{\Psi}^{(1)} A) = \langle\langle \Psi, A \otimes \mathbb{1}_{L_s^2(\mathbb{R}^{d(N-1)}, \mathbb{C})} \Psi \rangle\rangle \quad (1.4)$$

holds for all $\Psi \in L_s^2(\mathbb{R}^{dN}, \mathbb{C})$.

To account for the physical situation of a Bose-Einstein condensate, we assume complete condensation in the limit of large particle number N . Mathematically, this corresponds to convergence

$$\lim_{N \rightarrow \infty} \gamma_{\Psi_0}^{(1)} = |\varphi_0\rangle\langle\varphi_0| \quad (1.5)$$

in trace norm for some $\varphi_0 \in L^2(\mathbb{R}^2, \mathbb{C})$, $\|\varphi_0\| = 1$. φ_0 is then called the wavefunction of the condensate. Note that convergence in trace norm at time $t = 0$ implies

$$\lim_{N \rightarrow \infty} \text{tr}(\gamma_{\Psi_0}^{(1)} A) = \langle\varphi_0, A\varphi_0\rangle, \quad (1.6)$$

with $A \in \mathcal{B}(L^2(\mathbb{R}^d, \mathbb{C}))$, since $|\text{tr}(AB)| \leq \|A\|_{\text{op}} \text{tr}|B|$ holds for all $A, B \in \mathcal{B}(L^2(\mathbb{R}^d, \mathbb{C}))$, with B being trace class.

The general aim of this thesis is to prove persistence of condensation over time t . More precisely, we show the existence of a condensate wave function φ_t , such that the convergence $\gamma_{\Psi_t}^{(1)} \rightarrow |\varphi_t\rangle\langle\varphi_t|$ holds in trace norm. For the systems studied in this thesis, the effective function φ_t is given by a cubic nonlinear Schrödinger equation. The evolution of Ψ_t can therefore be approximated by the evolution of φ_t at the level of reduced density matrices. We will be concerned with interaction potentials $V^{(N)}$ which may be partly or purely attractive. In general, the dynamics of systems with attractive self-interaction may be unstable, resulting in a dynamical collapse. This is reflected by a blow-up of the effective equation φ_t . To prevent this type of effect, we will impose certain restrictions on the interaction which impose stability of second kind of the Hamiltonian H . The precise class of potentials will be discussed in detail in the respective chapters.

In the following, we will present these results:

- (a) The derivation of the two dimensional nonlinear Schrödinger and the two dimensional Gross-Pitaevskii equation.
- (b) The derivation of the three dimensional Gross-Pitaevskii equation for a class of non purely positive potentials.
- (c) The derivation of the two dimensional nonlinear Schrödinger equation for purely attractive interactions.

We will now give an overview on our results.

(a) In Chapter 3 we study a two dimensional system of N bosons. The potential $V^{(N)}$, as defined in the Hamiltonian (1.2), will be given as follows:

- We consider the interaction potential to be given by $e^{2N}V(e^N x)$, where $V \in L^\infty(\mathbb{R}^2, \mathbb{R})$ is a compactly supported and spherically symmetric potential. We choose V from a class of potentials which may have a sufficiently small attractive part.
- We consider the interaction potential to be given by $N^{-1+2\beta}W(N^\beta x)$, for $\beta > 0$. Again, $W \in L^\infty(\mathbb{R}^2, \mathbb{R})$ is compactly supported, spherically symmetric. We further assume the operator inequality $-(1-\epsilon)\Delta + \frac{1}{2}W \geq 0$ to hold on $L^2(\mathbb{R}^2, \mathbb{C})$ for some $0 < \epsilon < 1$.

Note that both scalings correspond to a system where strong but rare collisions are predominant. Under some assumptions on the initial wavefunction Ψ_0 , we prove that the time evolved reduced density matrix $\gamma_{\Psi_t}^{(1)}$ converges to $|\varphi_t\rangle\langle\varphi_t|$ in trace norm as $N \rightarrow \infty$ with convergence rate of order $N^{-\eta}$ for some $\eta > 0$. φ_t solves the nonlinear Schrödinger equation

$$i\partial_t\varphi_t = (-\Delta + A_t)\varphi_t + b|\varphi_t|^2\varphi_t \quad (1.7)$$

with initial datum φ_0 . For potentials which scale like $N^{-1+2\beta}W(N^\beta x)$, the coupling constants b is given by $b = \int_{\mathbb{R}^2} d^2x W(x)$. This can be motivated heuristically using a law of large number argument, see Chapter 3 for a detailed discussion.

The exponential scaling $e^{2N}V(e^N x)$ has to be treated separately. For a potential V with non-zero scattering length, the coupling constant b is given by $b = 4\pi$, regardless of the shape of the interaction V . This interesting effect only occurs in two spatial dimensions. We will explain in Chapter 3 why the existence of a short scale correlation structure present in Ψ_t accounts for this special behavior.

(b) In Chapter 4 we analyze the dynamics of a three dimensional Bose Einstein condensate in the so-called Gross-Pitaevskii regime. The time-dependent Hamiltonian H will be defined as

$$H = -\sum_{j=1}^N \Delta_j + N^2 \sum_{1 \leq j < k \leq N} V(N(x_j - x_k)) + \sum_{j=1}^N A_t(x_j). \quad (1.8)$$

We will prove persistence of condensation of Ψ_t for a class of potentials V which are not assumed to be nonnegative everywhere, but may have an attractive part. The detailed assumptions on V are listed in Assumption 4.2.3.

The condensate wave function of the system is given by the nonlinear Gross-Pitaevskii equation

$$i\partial_t\varphi_t = (-\Delta + A_t)\varphi_t + 8\pi a|\varphi_t|^2\varphi_t \quad (1.9)$$

with initial datum φ_0 . Here, a denotes the scattering length of the potential $\frac{1}{2}V$. We provide a derivation of the convergence of the reduced density matrix $\gamma_{\Psi_t}^{(1)}$ against the projection onto φ_t in trace norm as $N \rightarrow \infty$. Note that the class of potentials V we consider in this thesis is such that the scattering length a of V is nonnegative.

(c) In Chapter 5 we consider a two dimensional system of N bosons with strong, but short range interaction. The interaction potential of the system is given by $N^{-1+2\beta}W(N^\beta x)$. In contrast to (a), W may be chosen to be purely attractive¹. A system of N interacting, mutually attracting particles might be prone to dynamical collapse. This might be especially the case the bigger β is chosen, since then the interaction gets more singular. We therefore assume stability of second kind of H , i.e. $H \geq -CN$. We will see in Chapter 5 that this implies $\int_{\mathbb{R}^2} d^2x |W^-(x)| < a^*$, where W^- denotes the negative part of W and $a^* > 0$ denotes the optimal constant of the Gagliardo-Nirenberg inequality

$$\left(\int_{\mathbb{R}^2} d^2x |\nabla u(x)|^2 \right) \left(\int_{\mathbb{R}^2} d^2y |u(y)|^2 \right) \geq \frac{a^*}{2} \left(\int_{\mathbb{R}^2} d^2x |u(x)|^4 \right). \quad (1.10)$$

Under some additional assumptions on Ψ_0 , we then prove for $0 < \beta < 1$ convergence of $\gamma_{\Psi_t}^{(1)}$ to $|\varphi_t\rangle\langle\varphi_t|$ in trace norm as $N \rightarrow \infty$, where φ_t fulfills the nonlinear Schrödinger Equation (1.7) with $b = \int_{\mathbb{R}^2} d^2x W(x)$. In addition, for external potentials $A_t \in L^p(\mathbb{R}^2, \mathbb{R})$, with $p \in]2, \infty]$, we are able to show convergence in Sobolev trace norm, that is,

$$\lim_{N \rightarrow \infty} \text{Tr} \left| \sqrt{1 - \Delta} (\gamma_{\Psi_t}^{(1)} - |\varphi_t\rangle\langle\varphi_t|) \sqrt{1 - \Delta} \right| = 0. \quad (1.11)$$

Our proofs rely on a general method that is based on the idea of counting the rate of particles which leave the condensate over time. If it is possible to show that this rate is small, it can be inferred that the system can be described in terms of an effective condensate wave function φ_t . The idea of counting was developed in [61]. We will introduce the mathematical framework behind this idea in the next chapter.

Style of Writing:

The first person plural will be used throughout the work, as it is common in scientific writing. Chapters 3, 4 and 5 are written such that they can be read independently for most parts. Chapter 4 contains certain Lemmata which will be used in Chapter 3.

Note that certain mathematical objects may be defined differently from chapter to chapter. For example, the letter a denotes the scattering length of the potential $\frac{1}{2}V$ in Chapter 3 (see Lemma 3.3.2) and in Chapter 4 (see Eq. (4.30)), whereas a denotes the integral over W in Chapter 5. The specific changes in notation are minor and will be introduced at the beginning of each chapter. We also comment on the notation used throughout this work in 2.0.13.

¹ In two dimensions, it is well known that the operator inequality $-\Delta + \frac{1}{2}W \geq 0$ implies $\int_{\mathbb{R}^2} W(x) d^2x \geq 0$, since otherwise the operator $-\Delta + \frac{1}{2}W$ has at least one bound state with negative energy. Therefore, it is not possible to choose a purely attractive potential in part (a). We refer the reader to [13] for a nice discussion about this topic.

Chapter 2

Definition of the counting measure

In the following, we define several important concepts which make the idea of counting particles outside of the condensate precise. These concepts are well known within the literature and were introduced in [61].

Let \mathfrak{h} denote a separable Hilbert space. \mathfrak{h} corresponds to the one-particle sector of our system. N bosons are subsequently described on the Hilbert space $\mathcal{H}_s = \otimes_s^N \mathfrak{h}$. The subscript s denotes the symmetric tensor product, see e.g. [68] for a concise definition. We also define $\mathcal{H} = \otimes^N \mathfrak{h}$.

Notation 2.0.1 *In this thesis, we will work with the Hilbert spaces $\mathfrak{h} = L^2(\mathbb{R}^d, \mathbb{C})$; $d \in \{2, 3\}$, which in turn implies the identification*

$$\mathcal{H}_s = L_s^2(\mathbb{R}^{dN}, \mathbb{C}).$$

In particular, $L_s^2(\mathbb{R}^{dN}, \mathbb{C})$ denotes the set of all $\Psi(x_1, \dots, x_N) \in L^2(\mathbb{R}^{dN}, \mathbb{C})$ which are symmetric w.r.t. the pairwise permutation of the variables x_1, \dots, x_N ; $x_i \in \mathbb{R}^d$.

We will denote by $\|\cdot\|_p$, with $1 \leq p \leq \infty$, the L^p -norm on the appropriate Hilbert space. Moreover, the notation $\|\cdot\|$ will be used for the L^2 -norm. We denote by $\langle\langle \cdot, \cdot \rangle\rangle$ the scalar product on \mathcal{H} and by $\langle \cdot, \cdot \rangle$ the scalar product on the one-particle Hilbert space \mathfrak{h} .

Definition 2.0.2 *Let $\varphi \in \mathfrak{h}$ with $\|\varphi\| = 1$.*

(a) *Define $\mathcal{P}^\varphi : \mathcal{H} \rightarrow \mathfrak{h}$ as the projection onto φ . Let $1 \leq j \leq N$ and define the projectors $p_j^\varphi : \mathcal{H} \rightarrow \mathcal{H}$ and $q_j^\varphi : \mathcal{H} \rightarrow \mathcal{H}$ as*

$$p_j^\varphi = \underbrace{\mathbb{1}_{\mathfrak{h}} \otimes \cdots \otimes \mathbb{1}_{\mathfrak{h}}}_{j-1 \text{ times}} \otimes \mathcal{P}^\varphi \otimes \underbrace{\mathbb{1}_{\mathfrak{h}} \otimes \cdots \otimes \mathbb{1}_{\mathfrak{h}}}_{N-j \text{ times}},$$

$$q_j^\varphi = \mathbb{1}_{\mathcal{H}} - p_j^\varphi.$$

(b) *Let $0 \leq k \leq N$ and define the orthogonal projector $P_k^\varphi : \mathcal{H} \rightarrow \mathcal{H}$ as*

$$P_k^\varphi = \left(\prod_{j=1}^k q_j^\varphi \prod_{l=k+1}^N p_l^\varphi \right)_s =: \sum_{\substack{\vec{s} \in \{0,1\}^N \\ \sum_{i=1}^N s_i = k}} \prod_{j=1}^N (p_j^\varphi)^{1-s_j} (q_j^\varphi)^{s_j}.$$

For negative k and $k > N$, we define $P_k^\varphi = 0$.

(c) Let $m : \mathbb{N}_0 \rightarrow \mathbb{R}_0^+$ and define the operators $\widehat{m}^\varphi : \mathcal{H} \rightarrow \mathcal{H}$ as

$$\widehat{m}^\varphi = \sum_{j=0}^N m(j) P_j^\varphi, \quad \widehat{m}_d^\varphi = \sum_{j=-d}^{N-d} m(j+d) P_j^\varphi. \quad (2.1)$$

The function $m : \mathbb{N}_0 \rightarrow \mathbb{R}_0^+$ will be called a weight function.

Remark 2.0.3 For $\mathcal{H} = L^2(\mathbb{R}^{dN}, \mathbb{C})$, $d \in \mathbb{N}$, we may express

$$p_j^\varphi \Psi = \varphi(x_j) \int \varphi^*(\tilde{x}_j) \Psi(x_1, \dots, \tilde{x}_j, \dots, x_N) d^d \tilde{x}_j.$$

We will also use, with a slight abuse of notation, the bra-ket notation $p_j^\varphi = |\varphi(x_j)\rangle\langle\varphi(x_j)|$.

Remark 2.0.4 The definition of the projector $P_k^\varphi : \mathcal{H} \rightarrow \mathcal{H}$ corresponds to a decomposition of a wavefunction $\Psi \in \mathcal{H}_s$ into different excitation sectors. To be more precise, let $\mathfrak{h}_{\text{excitations}}$ be the orthogonal complement of the closed subspace $\{\varphi\}$ of \mathfrak{h} , that is $\mathfrak{h}_{\text{excitations}} = \{\varphi\}^\perp$. The wavefunction $P_k^\varphi \Psi$ with $\Psi \in \mathcal{H}_s$ can then be expressed as

$$P_k^\varphi \Psi = \varphi^{\otimes(N-k)} \otimes_s \chi_k.$$

with $\chi_k \in \otimes_s^k \mathfrak{h}_{\text{excitations}}$. In other words, P_k^φ projects onto the subspace with exactly $N - k$ particles in the state φ . Using

$$\sum_{k=0}^N P_k^\varphi = \mathbb{1}_{\mathcal{H}},$$

(see below for a proof), it is possible to decompose

$$\Psi = \sum_{k=0}^N P_k^\varphi \Psi = \sum_{k=0}^N \varphi^{\otimes(N-k)} \otimes_s \chi_k.$$

This decomposition into different excitation sectors was used in a series of papers, see e.g. [8, 9, 44] and references therein. For certain systems, it is possible to derive a Bogoliubov-type evolution equation for $(\chi_k)_{0 \leq k \leq N}$, see e.g. [51, 55] for a detailed discussion.

The operator \widehat{m}^φ will be used to count the number of particles which leave the condensate over time. To be more precise, for a suitable chosen weight function m , the functional $\langle\langle \Psi, \widehat{m}^\varphi \Psi \rangle\rangle$ will be a measure on the purity of the condensate. In order to make this idea precise, we will list certain lemmata which are needed in the next chapters. These lemmata are well known in the literature and can e.g. be found in [60].

Lemma 2.0.5 Let $\varphi \in \mathfrak{h}$ with $\|\varphi\| = 1$ and let $p_k = p_k^\varphi, P_k = P_k^\varphi$ and $\widehat{m} = \widehat{m}^\varphi$ be defined as in Definition 2.0.2.

(a) For any weights $m, r : \mathbb{N}_0 \rightarrow \mathbb{R}_0^+$ the commutation relations

$$\widehat{m}\widehat{r} = \widehat{m}\widehat{r} = \widehat{r}\widehat{m} \quad \widehat{m}p_j = p_j\widehat{m} \quad \widehat{m}q_j = q_j\widehat{m} \quad \widehat{m}P_k = P_k\widehat{m}$$

hold.

(b) $(P_k)_{0 \leq k \leq N}$ is a partition of identity, i.e.

$$\sum_{k=0}^N P_k = \mathbb{1}_{\mathcal{H}}.$$

(c) Let $n : \mathbb{N}_0 \rightarrow \mathbb{R}_0^+$ be given by $n(k) = \sqrt{k/N}$. Then,

$$(\widehat{n})^2 = \frac{1}{N} \sum_{j=1}^N q_j. \quad (2.2)$$

(d) Let $A_k : \mathcal{D}(A_k) \subset \mathfrak{h}^{\otimes k} \rightarrow \mathfrak{h}^{\otimes k}$ be a densely defined operator such that $\forall i \in \{1, \dots, k\} \forall \eta \in \mathcal{D}(A_k) : p_i \eta \in \mathcal{D}(A_k)$. Define $A = A_k \otimes \mathbb{1}_{\mathfrak{h}^{\otimes(N-k)}}$. Let $(s_1, \dots, s_k) \in \{0, 1\}^k$ with $\sum_{j=1}^k s_j = s$ and let $Q_s = \prod_{m=1}^k (p_i^{1-s_m} q_i^{s_m})$. Then, for any weight $m : \mathbb{N}_0 \rightarrow \mathbb{R}_0^+$, for $i, j \in \{1, \dots, k\}$

$$\widehat{m}Q_j A Q_k = Q_j A Q_k \widehat{m}_{j-k},$$

(e) Let $\mathfrak{h} = L^2(\mathbb{R}^d, \mathbb{C})$ for $d \in \mathbb{N}$. Let $m : \mathbb{N}_0 \rightarrow \mathbb{R}_0^+$ and let $f \in L^\infty(\mathbb{R}^{2d}, \mathbb{R})$. Define $Q_0 = p_1 p_2$, $Q_1 \in \{p_1 q_2, q_1 p_2\}$ and $Q_2 = q_1 q_2$. Then, for $j, k \in \{0, 1, 2\}$,

$$\widehat{m}Q_j f(x_1, x_2) Q_k = Q_j f(x_1, x_2) \widehat{m}_{j-k} Q_k.$$

Furthermore, if $\varphi \in H^1(\mathbb{R}^d, \mathbb{C})$ holds, we then obtain for $j, k \in \{0, 1\}$

$$\widehat{m}\widetilde{Q}_j \nabla_1 \widetilde{Q}_k = \widetilde{Q}_j \nabla_1 \widehat{m}_{j-k} \widetilde{Q}_k,$$

where $\widetilde{Q}_0 = p_1$ and $\widetilde{Q}_1 = q_1$.

(f) Let $\mathfrak{h} = L^2(\mathbb{R}^d, \mathbb{C})$ for $d \in \mathbb{N}$. Let $m : \mathbb{N}_0 \rightarrow \mathbb{R}_0^+$ and let $f \in L^\infty(\mathbb{R}^{2d}, \mathbb{C})$. Then,

$$[f(x_1, x_2), \widehat{m}] = [f(x_1, x_2), p_1 p_2 (\widehat{m} - \widehat{m}_2) + (p_1 q_2 + q_1 p_2) (\widehat{m} - \widehat{m}_1)].$$

(g) Let $\mathfrak{h} = L^2(\mathbb{R}^d, \mathbb{C})$ for $d \in \mathbb{N}$ and let $f \in L^1(\mathbb{R}^d, \mathbb{C})$, $g \in L^2(\mathbb{R}^d, \mathbb{C})$. Then,

$$\|p_j f(x_j - x_k) p_j\|_{op} \leq \|f\|_1 \|\varphi\|_\infty^2, \quad (2.3)$$

$$\|p_j g^*(x_j - x_k)\|_{op} = \|g(x_j - x_k) p_j\|_{op} \leq \|g\| \|\varphi\|_\infty, \quad (2.4)$$

$$\|\varphi(x_j)\langle \nabla_j \varphi(x_j) | h^*(x_j - x_k)\|_{op} = \|h(x_j - x_k) \nabla_j p_j\|_{op} \leq \|h\| \|\nabla \varphi\|_\infty. \quad (2.5)$$

Proof:

- (a) follows immediately from Definition 2.0.2, using that p_j and q_j are orthogonal projectors.
- (b) With the definition of P_k , we obtain

$$\begin{aligned} \sum_{k=0}^N P_k &= \sum_{k=0}^N \sum_{\substack{\vec{s} \in \{0,1\}^N \\ \sum_{i=1}^N s_i = k}} \prod_{j=1}^N (p_j)^{1-s_j} (q_j)^{s_j} \\ &= \prod_{n=1}^N (p_n + q_n) = \mathbb{1}_{\mathcal{H}}. \end{aligned}$$

- (c) With $(q_j)^2 = q_j$ and $q_j p_j = 0$, it follows

$$\sum_{j=1}^N q_j = \sum_{j=1}^N q_j \sum_{k=0}^N P_k = \sum_{k=0}^N \sum_{j=1}^N q_j P_k = \sum_{k=0}^N k P_k = N \widehat{n}^2 = N \widehat{n}^2.$$

- (d) First note that for $l \in \{0, \dots, N\}$ and $j \in \{0, \dots, k\}$, we obtain

$$\begin{aligned} Q_j P_l &= Q_j \sum_{\substack{\vec{s} \in \{0,1\}^N \\ \sum_{i=1}^N s_i = l}} \prod_{h=1}^N (p_h)^{1-s_h} (q_h)^{s_h} \\ &= Q_j \sum_{\substack{\vec{s} \in \{0,1\}^N \\ \sum_{i=1}^N s_i = l}} \prod_{h=1}^N (p_h)^{1-s_h} (q_h)^{s_h} \delta_{\sum_{m=k+1}^N s_m, l-j}. \end{aligned}$$

In other words, in the equation above, the number of q_h with $h \leq k$ is j and the number of q_h with $h > k$ is given by $l - j$. Defining the projector

$$\tilde{P}_{l-j} = \sum_{\substack{\vec{s} \in \{0,1\}^N \\ \sum_{i=k+1}^N s_i = l-j}} \prod_{h=k+1}^N (p_h)^{1-s_h} (q_h)^{s_h},$$

we obtain

$$Q_j P_l = Q_j \otimes \tilde{P}_{l-j}.$$

For $l, m \in \{0, \dots, N\}$, we may therefore write

$$P_l Q_j A Q_r P_m = (Q_j A Q_k) \otimes (\tilde{P}_{l-j} \tilde{P}_{m-r}) = \delta_{l-j, m-r} (Q_j A Q_k) \otimes \tilde{P}_{l-j}.$$

As a consequence, the identity

$$P_l Q_j A Q_r P_m = \delta_{l-j, m-r} Q_j A Q_r P_m = \delta_{l-j, m-r} P_l Q_j A Q_r$$

holds. Let us now consider

$$\begin{aligned} \widehat{m} Q_j A Q_k &= \sum_{i=0}^N m(i) P_i Q_j A Q_k = Q_j A Q_k \sum_{i=0}^N m(i) P_{i-j+k} \\ &= Q_j A Q_k \sum_{i=-j+k}^{N-j+k} m(i+j-k) P_i = Q_j A q_k \widehat{m}_{j-k}. \end{aligned}$$

- (e) This is a direct consequence from (d).
- (f) By virtue of (e), we obtain the following identity

$$\begin{aligned} &[f(x_1, x_2), \widehat{m}] - [f(x_1, x_2), p_1 p_2 (\widehat{m} - \widehat{m}_2) + p_1 q_2 (\widehat{m} - \widehat{m}_1) + q_1 p_2 (\widehat{m} - \widehat{m}_1)] \\ &= [f(x_1, x_2), q_1 q_2 \widehat{m}] + [f(x_1, x_2), p_1 p_2 \widehat{m}_2 + p_1 q_2 \widehat{m}_1 + q_1 p_2 \widehat{m}_1]. \end{aligned} \quad (2.6)$$

We multiply the right hand side with $p_1 p_2$ from the left which yields to

$$\begin{aligned} &p_1 p_2 f(x_1, x_2) q_1 q_2 \widehat{m} + p_1 p_2 f(x_1, x_2) p_1 p_2 \widehat{m}_2 - p_1 p_2 \widehat{m}_2 f(x_1, x_2) \\ &+ p_1 p_2 f(x_1, x_2) p_1 q_2 \widehat{m}_1 + p_1 p_2 f(x_1, x_2) q_1 p_2 \widehat{m}_1 \\ &= p_1 p_2 \widehat{m}_2 f(x_1, x_2) q_1 q_2 + p_1 p_2 \widehat{m}_2 f(x_1, x_2) p_1 p_2 - p_1 p_2 \widehat{m}_2 f(x_1, x_2) \\ &+ p_1 p_2 \widehat{m}_2 f(x_1, x_2) p_1 q_2 + p_1 p_2 \widehat{m}_2 f(x_1, x_2) q_1 p_2 \\ &= 0. \end{aligned}$$

Multiplying (2.6) with $p_1 q_2$ from the left one gets

$$\begin{aligned} &p_1 q_2 f(x_1, x_2) q_1 q_2 \widehat{m} + p_1 q_2 f(x_1, x_2) p_1 p_2 \widehat{m}_2 + p_1 q_2 f(x_1, x_2) p_1 q_2 \widehat{m}_1 \\ &+ p_1 q_2 f(x_1, x_2) q_1 p_2 \widehat{m}_1 - p_1 q_2 \widehat{m}_1 f(x_1, x_2). \end{aligned}$$

Using (e), the latter is zero. Also multiplying with $q_1 p_2$ yields zero due to symmetry in interchanging x_1 with x_2 . Multiplying (2.6) with $q_1 q_2$ from the left one gets

$$\begin{aligned} &q_1 q_2 f(x_1, x_2) \widehat{m} q_1 q_2 - q_1 q_2 \widehat{m} f(x_1, x_2) + q_1 q_2 f(x_1, x_2) p_1 p_2 \widehat{m}_2 + \\ &q_1 q_2 f(x_1, x_2) p_1 q_2 \widehat{m}_1 + q_1 q_2 f(x_1, x_2) q_1 p_2 \widehat{m}_1 \end{aligned}$$

which is again zero and so is (2.6).

- (g) First note that, for bounded operators A, B , $\|AB\|_{\text{op}} = \|B^* A^*\|_{\text{op}}$ holds, where A^* is the adjoint operator of A . To show (2.3), note that

$$p_j f(x_j - x_k) p_j = p_j (f \star |\varphi|^2)(x_k). \quad (2.7)$$

It follows that

$$\|p_j f(x_j - x_k) p_j\|_{\text{op}} \leq \|f\|_1 \|\varphi\|_\infty^2.$$

For (2.4) we write

$$\begin{aligned} \|g(x_j - x_k) p_j\|_{\text{op}}^2 &= \sup_{\|\Psi\|=1, \Psi \in \mathcal{H}} \|g(x_j - x_k) p_j \Psi\|^2 = \\ &= \sup_{\|\Psi\|=1, \Psi \in \mathcal{H}} \langle\langle \Psi, p_j |g(x_j - x_k)|^2 p_j \Psi \rangle\rangle \\ &\leq \|p_j |g(x_j - x_k)|^2 p_j\|_{\text{op}}. \end{aligned}$$

With (2.3) we get (2.4). For (2.5) we use

$$\begin{aligned} \|g(x_j - x_k) \nabla_j p_j\|_{\text{op}}^2 &= \sup_{\|\Psi\|=1, \Psi \in \mathcal{H}} \langle\langle \Psi, p_j (|g|^2 * |\nabla \varphi|^2)(x_k) \Psi \rangle\rangle \leq \| |g|^2 * |\nabla \varphi|^2 \|_\infty \\ &\leq \|g\|^2 \|\nabla \varphi\|_\infty^2. \end{aligned}$$

□

Next, we will consider wavefunctions $\Psi \in \mathcal{H}$ which are not symmetric w.r.t. to all arguments. As an example, the reader may think of $p_1^\varphi q_2^\varphi \Psi$, with $\Psi \in \mathcal{H}_s$.

Definition 2.0.6 Let $\sigma \in S_N$ be a permutation of the numbers $(1, \dots, N)$ and define $P_\sigma : \mathcal{H} \rightarrow \mathcal{H}$ by its action on tensor products

$$P_\sigma \varphi_1 \otimes \dots \varphi_N = \varphi_{\sigma_1} \otimes \dots \otimes \varphi_{\sigma_N}$$

with $\varphi_k \in \mathfrak{h}$, $k \in \{1, \dots, N\}$. Let $\mathcal{M} \subset \{1, 2, \dots, N\}$ and define $S_{N, \mathcal{M}} = \{\sigma \in S_N \mid \sigma_k = k \forall k \in \mathcal{M}\}$. Then $\mathcal{H}_\mathcal{M} \subset \mathcal{H}$ is defined as

$$\mathcal{H}_\mathcal{M} = \{\Psi \in \mathcal{H} \mid P_\sigma \Psi = \Psi \forall \sigma \in S_{N, \mathcal{M}}\}.$$

This readily yields to

Lemma 2.0.7 Let $f : \mathbb{N}_0 \rightarrow \mathbb{R}_0^+$ and let $\mathcal{M}_a \subset \{1, 2, \dots, N\}$ with $1 \in \mathcal{M}_a$, as well as $\mathcal{M}_b \subset \{1, 2, \dots, N\}$ with $1, 2 \in \mathcal{M}_b$. Then,

$$\|\widehat{f} q_1 \Psi\|^2 \leq \frac{N}{|\mathcal{M}_a|} \|\widehat{f} \widehat{n} \Psi\|^2 \quad \text{for any } \Psi \in \mathcal{H}_{\mathcal{M}_a}, \quad (2.8)$$

$$\|\widehat{f} q_1 q_2 \Psi\|^2 \leq \frac{N^2}{|\mathcal{M}_b|(|\mathcal{M}_b| - 1)} \|\widehat{f}(\widehat{n})^2 \Psi\|^2 \quad \text{for any } \Psi \in \mathcal{H}_{\mathcal{M}_b}. \quad (2.9)$$

Proof: For $\Psi \in \mathcal{H}_{\mathcal{M}_a}$. (2.8) can be estimated by Lemma 2.0.5 (c) as

$$\begin{aligned} \|\widehat{f} \widehat{n} \Psi\|^2 &= \langle\langle \Psi, (\widehat{f})^2(\widehat{n})^2 \Psi \rangle\rangle = N^{-1} \sum_{k=1}^N \langle\langle \Psi, (\widehat{f})^2 q_k \Psi \rangle\rangle \\ &\geq N^{-1} \sum_{k \in \mathcal{M}_a} \langle\langle \Psi, (\widehat{f})^2 q_k \Psi \rangle\rangle = \frac{|\mathcal{M}_a|}{N} \langle\langle \Psi, (\widehat{f})^2 q_1 \Psi \rangle\rangle \\ &= \frac{|\mathcal{M}_a|}{N} \|\widehat{f} q_1 \Psi\|^2. \end{aligned}$$

Similarly, we obtain for $\Psi \in \mathcal{H}_{\mathcal{M}_b}$

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

which concludes the Lemma. \square

Corollary 2.0.8 *Let $A : \mathcal{D}(A) \subset \mathfrak{h} \rightarrow \mathfrak{h}$ and define $A_i = \underbrace{\mathbb{1}_{\mathfrak{h}} \otimes \cdots \otimes \mathbb{1}_{\mathfrak{h}}}_{i-1 \text{ times}} \otimes A \otimes \underbrace{\mathbb{1}_{\mathfrak{h}} \otimes \cdots \otimes \mathbb{1}_{\mathfrak{h}}}_{N-i \text{ times}}$.*

Let $\Psi \in \mathcal{H}_s$ such that $\|A_1 q_1 \Psi\| < \infty$. Then, for any weight $m : \mathbb{N}_0 \rightarrow \mathbb{R}_0^+$ which is monotone nondecreasing

$$\|A_1 \widehat{m} q_1 \Psi\| \leq 2 \|\widehat{m}\|_{op} \|A_1 q_1 \Psi\|, \quad (2.10)$$

$$\|A_1 \widehat{m} q_1 q_2 \Psi\| \leq C \|\widehat{m} \widehat{n}\|_{op} \|A_1 q_1 \Psi\|. \quad (2.11)$$

Remark 2.0.9 *We will mainly be concerned with $A = -i\nabla$ during the rest of this thesis.*

Proof: Using $p_1 + q_1 = \mathbb{1}_{\mathcal{H}}$ and triangle inequality,

$$\|A_1 \widehat{m} q_1 \Psi\| \leq \|p_1 A_1 \widehat{m} q_1 \Psi\| + \|q_1 A_1 \widehat{m} q_1 \Psi\|, \quad (2.12)$$

$$\|A_1 \widehat{m} q_1 q_2 \Psi\| \leq \|p_1 A_1 \widehat{m} q_1 q_2 \Psi\| + \|q_1 A_1 \widehat{m} q_1 q_2 \Psi\|. \quad (2.13)$$

With Lemma 2.0.5 (c) we get

$$(2.12) = \|\widehat{m}_1 p_1 A_1 q_1 \Psi\| + \|\widehat{m} q_1 A_1 q_1 \Psi\| \leq (\|\widehat{m}_1\|_{op} + \|\widehat{m}\|_{op}) \|A_1 q_1 \Psi\|.$$

Since $m(k)$ is monotone nondecreasing, we obtain $\|\widehat{m}_1\|_{op} = \|\widehat{m}\|_{op}$. Note that $p_1 A_1 q_1 \Psi \in \mathcal{H}_{\{1, \dots, N\} \setminus \{1\}}$. By Lemma 2.0.7 we obtain

$$\begin{aligned} (2.13) &= \|q_2 \widehat{m}_1 p_1 A_1 q_1 \Psi\| + \|q_2 \widehat{m} q_1 A_1 q_1 \Psi\| \\ &\leq \frac{N}{N-1} (\|\widehat{m}_1 \widehat{n}\|_{op} + \|\widehat{m} \widehat{n}\|_{op}) \|A_1 q_1 \Psi\|. \end{aligned}$$

Since $\sqrt{k} \leq \sqrt{k+1}$ for $k \geq 0$ it follows that the latter is bounded by

$$C(\|\widehat{m}_1 \widehat{n}_1\|_{op} + \|\widehat{m} \widehat{n}\|_{op}) \|A_1 q_1 \Psi\|.$$

Note that

$$\widehat{m}_1 \widehat{n}_1 = \widehat{m} \widehat{n}_1 = \sum_{j=0}^{N-1} m(j+1) n(j+1) P_j,$$

so that $\|\widehat{m}_1 \widehat{n}_1\|_{op} = \sup_{1 \leq k \leq N} \{m(k)n(k)\}$. Since $n(0) = 0$, we then obtain $\|\widehat{m}_1 \widehat{n}_1\|_{op} = \sup_{0 \leq k \leq N} \{m(k)n(k)\} = \|\widehat{m} \widehat{n}\|_{op}$ and the Corollary follows.

□

Lemma 2.0.10 *Let $\Omega, \chi \in \mathcal{H}_{\mathcal{M}}$ for some \mathcal{M} , let $1 \notin \mathcal{M}$ and $2, 3 \in \mathcal{M}$. Let $O_{j,k}$ be an operator acting on the j^{th} and k^{th} coordinate. Then*

$$|\langle\langle \Omega, O_{1,2}\chi \rangle\rangle| \leq \|\Omega\|^2 + |\langle\langle O_{1,2}\chi, O_{1,3}\chi \rangle\rangle| + (|\mathcal{M}|)^{-1}\|O_{1,2}\chi\|^2.$$

Proof: Using symmetry and Cauchy Schwarz, we get

$$\begin{aligned} |\langle\langle \Omega, O_{1,2}\chi \rangle\rangle| &= |\mathcal{M}|^{-1}|\langle\langle \Omega, \sum_{j \in \mathcal{M}} O_{1,j}\chi \rangle\rangle| \leq |\mathcal{M}|^{-1}\|\Omega\| \|\sum_{j \in \mathcal{M}} O_{1,j}\chi\| \\ &\leq \|\Omega\|^2 + |\mathcal{M}|^{-2} \left\| \sum_{j \in \mathcal{M}} O_{1,j}\chi \right\|^2. \end{aligned}$$

The second factor can be rewritten as

$$\begin{aligned} \left\| \sum_{j \in \mathcal{M}} O_{1,j}\chi \right\|^2 &= \langle\langle \sum_{j \in \mathcal{M}} O_{1,j}\chi, \sum_{k \in \mathcal{M}} O_{1,k}\chi \rangle\rangle \\ &\leq \sum_{j \in \mathcal{M}} |\langle\langle O_{1,j}\chi, O_{1,j}\chi \rangle\rangle| + \sum_{j \neq k \in \mathcal{M}} |\langle\langle O_{1,j}\chi, O_{1,k}\chi \rangle\rangle| \\ &\leq |\mathcal{M}| |\langle\langle O_{1,2}\chi, O_{1,2}\chi \rangle\rangle| + |\mathcal{M}|(|\mathcal{M}| - 1) |\langle\langle O_{1,2}\chi, O_{1,3}\chi \rangle\rangle|. \end{aligned}$$

□

Finally, we connect the functional $\langle\langle \Psi, \widehat{m}^\varphi \Psi \rangle\rangle$ to the convergence of the reduced density matrices. In particular, for a suitable chosen weight function, $\lim_{N \rightarrow \infty} \langle\langle \Psi, \widehat{m}^\varphi \Psi \rangle\rangle = 0$ implies $\lim_{N \rightarrow \infty} \gamma_\Psi^{(1)} = |\varphi\rangle\langle\varphi|$ in trace norm.

Lemma 2.0.11 *Let $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C})$, $\|\Psi\| = 1$ and let $\varphi \in L^2(\mathbb{R}^2, \mathbb{C})$, $\|\varphi\| = 1$. Let $m : \mathbb{N}_0 \rightarrow \mathbb{R}_0^+$ and define $\alpha(\Psi, \varphi) = \langle\langle \Psi, \widehat{m}^\varphi \Psi \rangle\rangle$. Assume the operator inequality*

$$\widehat{m}^\varphi \leq \frac{1}{N} \sum_{j=1}^N q_j^\varphi.$$

Then,

$$\lim_{N \rightarrow \infty} \alpha(\Psi, \varphi) = 0 \Leftrightarrow \lim_{N \rightarrow \infty} \gamma_\Psi^{(1)} = |\varphi\rangle\langle\varphi| \text{ in trace norm.}$$

Proof: For symmetric $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C})$, the operator inequality $\widehat{m}^\varphi \leq \frac{1}{N} \sum_{j=1}^N q_j^\varphi$ implies, together with the assumption on m , $0 \leq \langle\langle \Psi, \widehat{m}^\varphi \Psi \rangle\rangle \leq \langle\langle \Psi, q_1^\varphi \Psi \rangle\rangle$. The Lemma then follows from the estimate $\langle\langle \Psi, q_1^\varphi \Psi \rangle\rangle \leq \text{Tr}|\gamma_\Psi^{(1)} - |\varphi\rangle\langle\varphi|| \leq \sqrt{8\langle\langle \Psi, q_1^\varphi \Psi \rangle\rangle}$ which was proven in [34].

□

Remark 2.0.12 The convergence of $\gamma_{\Psi_t}^{(1)}$ to $|\varphi_t\rangle\langle\varphi_t|$ in trace norm is equivalent to convergence in operator norm and in Hilbert-Schmidt norm, since $|\varphi_t\rangle\langle\varphi_t|$ is a rank one projection [65]. Furthermore, the convergence of the one-particle reduced density matrix $\gamma_{\Psi_t}^{(1)} \rightarrow |\varphi_t\rangle\langle\varphi_t|$ in trace norm implies convergence of any k -particle reduced density matrix $\gamma_{\Psi_t}^{(k)}$ against $|\varphi_t^{\otimes k}\rangle\langle\varphi_t^{\otimes k}|$ in trace norm as $N \rightarrow \infty$ and k fixed, see for example [34]. Other equivalent definitions of asymptotic 100% condensation can be found in [48].

We will comment on the notation we will employ during the rest of this work.

Notation 2.0.13 (a) Throughout this thesis, hats $\hat{\cdot}$ will be used in the sense of Definition 2.0.2 (c). In the context of \hat{n}^φ , the label n will always be used for the function $n(k) = \sqrt{k/N}$.

- (b) For better readability, we will in general omit the upper index φ on p_j , q_j , P_j and $\hat{\cdot}$.
- (c) We will bound expressions which are uniformly bounded in N and t by some constant C . We will not distinguish constants appearing in a sequence of estimates, i.e. in $X \leq CY \leq CZ$ the constants may differ.
- (d) We will denote the operator norm defined for any linear operator $f : \mathcal{H} \rightarrow \mathcal{H}$ by

$$\|f\|_{op} = \sup_{\psi \in \mathcal{H}, \|\Psi\|=1} \|f\Psi\|.$$

- (e) We will denote for any multiplication operator $F : L^2(\mathbb{R}^d, \mathbb{C}) \rightarrow L^2(\mathbb{R}^d, \mathbb{C})$ the corresponding operator

$$\mathbb{1}_{L^2(\mathbb{R}^d, \mathbb{C})}^{\otimes(k-1)} \otimes F \otimes \mathbb{1}_{L^2(\mathbb{R}^d, \mathbb{C})}^{\otimes(N-k)} : L^2(\mathbb{R}^{dN}, \mathbb{C}) \rightarrow L^2(\mathbb{R}^{dN}, \mathbb{C})$$

acting on the N -particle Hilbert space by $F(x_k)$. In particular, we will use, for any $\Psi, \Omega \in L^2(\mathbb{R}^{dN}, \mathbb{C})$ the notation

$$\langle\langle \Omega, \mathbb{1}_{L^2(\mathbb{R}^d, \mathbb{C})}^{\otimes(k-1)} \otimes F \otimes \mathbb{1}_{L^2(\mathbb{R}^d, \mathbb{C})}^{\otimes(N-k)} \Psi \rangle\rangle = \langle\langle \Omega, F(x_k) \Psi \rangle\rangle.$$

In analogy, for any two-particle multiplication operator $K : L^2(\mathbb{R}^d, \mathbb{C})^{\otimes 2} \rightarrow L^2(\mathbb{R}^d, \mathbb{C})^{\otimes 2}$, we denote the operator acting on any $\Psi \in L^2(\mathbb{R}^{dN}, \mathbb{C})$ by multiplication in the variable x_i and x_j by $K(x_i, x_j)$. In particular, we denote

$$\langle\langle \Omega, K(x_i, x_j) \Psi \rangle\rangle = \int_{\mathbb{R}^{2N}} K(x_i, x_j) \Omega^*(x_1, \dots, x_N) \Psi(x_1, \dots, x_N) d^2x_1 \dots d^2x_N.$$

- (f) For any Hilbert space \mathcal{K} , we write 1 instead of $\mathbb{1}_{\mathcal{K}}$ in the following to denote the identity on \mathcal{K} .
- (g) Furthermore, define for any set $A \subset \mathbb{R}^{dN}$ the operator $\mathbb{1}_A : L^2(\mathbb{R}^{dN}, \mathbb{C}) \rightarrow L^2(\mathbb{R}^{dN}, \mathbb{C})$ as the projection onto the set A .

Chapter 3

Derivation of the Two Dimensional Gross-Pitaevskii Equation

Contributions of the author and Acknowledgments

This chapter presents joint work with Dr. Nikolai Leopold and Prof. Dr. Peter Pickl and resulted in the preprint [25]. The present chapter is an expanded version of this preprint and generalizes Theorem 3.2.5 to interaction potentials which are not assumed to be non-negative everywhere. The preprint was written by me. The contributions of the author of this thesis may be expected to consist of approximately sixty percent of the original project as presented in [25]. The strategy of the proof presented in this chapter is based on [60], where the three-dimensional Gross-Pitaevskii equation was derived.

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3.1 Introduction

This chapter deals with the effective dynamics of a two dimensional condensate of N interacting bosons. Fundamentally, the evolution of the system is described by a time-dependent wave-function $\Psi_t \in L_s^2(\mathbb{R}^{2N}, \mathbb{C})$, $\|\Psi_t\| = 1$. Assuming that $\Psi_0 \in H^2(\mathbb{R}^{2N}, \mathbb{C})$ holds, Ψ_t then solves the N -particle Schrödinger equation

$$i\partial_t \Psi_t = H_U \Psi_t \quad (3.1)$$

where the (non-relativistic) Hamiltonian $H_U : H^2(\mathbb{R}^{2N}, \mathbb{C}) \rightarrow L^2(\mathbb{R}^{2N}, \mathbb{C})$ is given by

$$H_U = - \sum_{j=1}^N \Delta_j + \sum_{1 \leq j < k \leq N} U(x_j - x_k) + \sum_{j=1}^N A_t(x_j). \quad (3.2)$$

In general, even for small particle numbers N , the evolution Equation (3.1) cannot be solved neither exactly nor numerically for Ψ_t . Nevertheless, for a certain class of scaled potentials U and certain initial conditions Ψ_0 it is possible to derive an approximate solution of (3.1) in the trace class topology of reduced density matrices. The picture we have in mind is the description of a Bose-Einstein condensate. Initially, one starts with the ground state of a trapped, dilute gas and then removes or changes the trap subsequently. In this chapter, we will consider two choices for the interaction potential U .

- Let $U(x) = V_N(x) = e^{2N}V(e^N x)$ for a compactly supported, spherically symmetric potential $V \in L_c^\infty(\mathbb{R}^2, \mathbb{R})$. Below, the exponential scaling of V_N will be explained in detail. Note that, in contrast to existing dynamical mean-field results, $\|V_N\|_1 = \mathcal{O}(1)$ does not decay like $1/N$. The interaction potential V is not assumed to be a nonnegative function, but may have small attractive part, see 3.2.3 for the detailed assumptions on V . We like to remark that the conditions imposed on V are due to a result of Jun Yin, see [72]. We provide a detailed discussion on these assumptions in Chapter 4. There, we also prove some important inequalities we need for the main result of this chapter. Note that the focus of this chapter lies on the correlation structure induced by V_N , as explained below. In order for the presentation not to be cluttered, we decided not to discuss Assumption 3.2.3 in this chapter, but rather refer the reader to Chapter 4.
- Let, for any fixed $\beta > 0$, $U(x) = W_\beta(x) = N^{-1+2\beta}W(N^\beta x)$ for a compactly supported, spherically symmetric, potential $W \in L_c^\infty(\mathbb{R}^2, \mathbb{R})$. This scaling of W_β can be motivated by formally imposing that that the total potential energy is of the same order as the total kinetic energy, namely of order N , if Ψ_0 is close to the ground state. We furthermore assume $-(1-\epsilon)\Delta + \frac{1}{2}W \geq 0$ as an operator inequality on $L^2(\mathbb{R}^2, \mathbb{C})$ for some $\epsilon > 0$. This condition is equivalent to the condition that the operator $-(1-\epsilon)\Delta + \frac{1}{2}W$ has no bound state. It is well known that the operator inequality stated above cannot be fulfilled for potentials W which satisfy $\int_{\mathbb{R}^2} W(x)d^2x < 0$, see e.g. [13]. Hence, W must have a sufficiently large positive part. We will discuss potentials W which are nonpositive in Chapter 5.

Both the Assumption 3.2.3 on V , as well the operator inequality $-(1-\epsilon)\Delta + \frac{1}{2}W \geq 0$ are used in the following to prevent clustering of particles. In particular, these conditions imply $\|\nabla_1 \Psi_t\| \leq C$ uniformly in N , see Lemma 3.5.1. We will comment on the possible clustering of particles in more details in Chapter 4 and in Chapter 5.

Recall the definition of the one particle reduced density matrix $\gamma_{\Psi_0}^{(1)}$ of Ψ_0 with integral kernel

$$\gamma_{\Psi_0}^{(1)}(x, x') = \int_{\mathbb{R}^{2N-2}} \Psi_0^*(x, x_2, \dots, x_N) \Psi_0(x', x_2, \dots, x_N) d^2x_2 \dots d^2x_N.$$

To account for the physical situation of a Bose-Einstein condensate, we assume complete condensation in the limit of large particle number N . This amounts to assume that, for $N \rightarrow \infty$, $\gamma_{\Psi_0}^{(1)} \rightarrow |\varphi_0\rangle\langle\varphi_0|$ in trace norm for some $\varphi_0 \in L^2(\mathbb{R}^2, \mathbb{C})$, $\|\varphi_0\| = 1$. Our main goal is to show the persistence of condensation over time. This is of particular interest in

experiments if one switches off the trapping potential A_t and monitors the expansion of the condensate. We prove that the time evolved reduced density matrix $\gamma_{\Psi_t}^{(1)}$ converges to $|\varphi_t\rangle\langle\varphi_t|$ in trace norm as $N \rightarrow \infty$ with convergence rate of order $N^{-\eta}$ for some $\eta > 0$. φ_t then solves the nonlinear Schrödinger equation

$$i\partial_t\varphi_t = (-\Delta + A_t)\varphi_t + b_U|\varphi_t|^2\varphi_t =: h_{b_U}^{GP}\varphi_t \quad (3.3)$$

with initial datum φ_0 .

Depending on the interaction potential U , we obtain different coupling constants b_U . For $U = W_\beta$, we obtain $b_{W_\beta} = N \int_{\mathbb{R}^2} W_\beta(x) d^2x = \int_{\mathbb{R}^2} W(x) d^2x$. This result is already expected from a heuristic law of large numbers argument, see below. Also note, by the operator inequality $-\Delta + \frac{1}{2}V \geq 0$, it follows $b_{W_\beta} \geq 0$. Thus, the effective nonlinear Schrödinger equation is repulsive. This is also reflected by the fact that the inequality $-(1-\epsilon)\Delta + \frac{1}{2}W \geq 0$, with $\epsilon > 0$, implies the operator inequality $-\epsilon \sum_{k=1}^N \Delta_k \leq -\sum_{k=1}^N \Delta_k + \sum_{i < j}^N W_\beta(x_i - x_j)$, see Lemma 3.5.1. This inequality is crucial to bound $\|\nabla_1 \Psi_t\|$ uniformly in N and to hence prevents the possibility of a dynamical collapse. We will discuss this issue in much more detail both in Chapter 4 and in Chapter 5. In the latter chapter, we also discuss more general potentials W_β , $0 < \beta < 1$, which may be chosen to be purely attractive.

In the case $U = V_N$, we distinguish two cases. For a positive scattering length a of the potential $\frac{1}{2}V$ (see Section 3.3 for the definition of a), $b_{V_N} = 4\pi$ holds. If the scattering length a is zero, we obtain $b_{V_N} = 0$. Then, the evolution of condensate is according to the one-particle linear Schrödinger equation with external field A_t . Note that, in contrast to three-dimensional Bose gases, the scattering length a of the potential $\frac{1}{2}V$ is always nonnegative, see Section 3.3.

In the case that the time evolution of Ψ_t is generated by H_{V_N} it is interesting to note that the effective evolution equation of φ_t does not depend on the scattering length a , apart from the fact that one must distinguish the cases $a > 0$ and $a = 0$. This contrasts the three dimensional case, where the correct mean field coupling is given by $8\pi a_{3D}$, a_{3D} denoting the scattering length of the potential in three dimensions. The universal coupling 4π in the case of a positive scattering length is known within the physical literature, see e.g. (30) and (A3) in [15] (note that $\hbar = 1, m = \frac{1}{2}$ in our choice of coordinates). Actually, our dynamical result complements a more general theory describing the ground state properties of dilute Bose gases. It was shown in [42] that for such a gas with repulsive interaction $V \geq 0$, the ground state energy per particle is to leading order given by either the Gross-Pitaevskii energy functional with coupling parameter $8\pi/|\ln(\bar{\rho}a^2)|$ or a Thomas-Fermi type functional. Here, $\bar{\rho}$ denotes the mean density of the gas, see Equation (1.6) in [42] for a precise definition. The authors prove further that only if $N/|\ln(\bar{\rho}a^2)| = \mathcal{O}(1)$ holds, one obtains the Gross-Pitaevskii regime. This directly implies that scattering length of the interaction potential needs to have an exponential decrease in N . In our case, the scattering length of the potential $\frac{1}{2}V_N$ is given by ae^{-N} , a denoting the scattering length of $\frac{1}{2}V$. The mean density of the system we consider is of order one, i.e. $\bar{\rho} = \mathcal{O}(1)$. This yields $8\pi N/|\ln(\bar{\rho}(e^{-N}a)^2)| \approx 4\pi$ which is in agreement with our findings. It should be

pointed out that there has been some debate about the question whether two dimensional Bose-Einstein condensation can be observed experimentally. This amounts to the question whether condensation takes place for temperatures $T > 0$. For an ideal, noninteracting gas in box, the standard grand canonical computation for the critical temperature T_c of a Bose-Einstein condensate shows that there is no condensation for $T > 0$. For trapped, noninteracting Bosons in a confining power-law potential, the findings in [3] however show that in that case $T_c > 0$ holds. Finally, it was proven in [39] that $\gamma_{\Psi}^{(1)}$ converges to $|\varphi\rangle\langle\varphi|$ in trace norm if Ψ the ground state of H_{V_N} and φ is the ground state of the Gross-Pitaevskii energy functional, see (3.5). The assumptions made in the paper are that and the external potential A tends to $+\infty$ as $|x| \rightarrow \infty$ and the interaction potential V is nonnegative. It is also remarked that one does not observe 100 % condensation in the ground state of a interacting homogenous system. The emergence of 100 % Bose-Einstein condensation as a ground state phenomena thus highly depends on the particular physical system one considers. Our approach is the following: Initially, we assume the convergence of $\gamma_{\Psi_0}^{(1)}$ to $|\varphi_0\rangle\langle\varphi_0|$. We then show the persistence this condensation for time scales of order one. Our assumption is thus in agreement with the findings in [39]. We like to remark that the two dimensional Thomas-Fermi regime could be observed experimentally [23].

Next, we want to explain how the different coupling constants b_U are obtained in the dynamical setting. For this, we first recall known results from the three dimensional Bose gas. There, one considers the interaction potential to be given by $V_{\beta}(x) = N^{-1+3\beta}V(N^{\beta}x)$ for $0 \leq \beta \leq 1$. For $0 < \beta < 1$, one obtains the cubic nonlinear Schrödinger equation with coupling constant $\|V\|_1$. This can be seen as a singular mean-field limit, where the full interaction is replaced by its corresponding mean value $\int_{\mathbb{R}^3} d^3y N^{3\beta}V(N^{\beta}(x-y))|\varphi_t(y)|^2 \rightarrow \|V\|_1|\varphi_t(x)|^2$. For $\beta = 1$, however, the system develops correlations between the particles which cannot be neglected. As already mentioned, the correct mean field coupling is then given by $8\pi a_{3D}$. This is different for a two dimensional condensate. Let us first explain, why the short scale correlation structure is negligible if the potential is given by $W_{\beta}(x) = N^{-1+2\beta}W(N^{\beta}x)$ for any $\beta > 0$. Assuming that the energy of Ψ_t is comparable to the ground state energy, the wave function will develop short scale correlations between the particles. One may heuristically think of Ψ_t of Jastrow-type, i.e. $\Psi_t(x_1, \dots, x_N) \approx \prod_{i < j} F(x_i - x_j) \prod_{k=1}^N \varphi_t(x_k)$ ¹. The function F accounts for the pair correlations between the particles at short scales of order $N^{-\beta}$. It is well known that the correlation function F should be described by the zero energy scattering state $j_{N,R}$ of the potential W_{β} , where $j_{N,R}$ satisfies

$$\begin{cases} \left(-\Delta_x + \frac{1}{2}W_{\beta}(x)\right) j_{N,R}(x) = 0, \\ j_{N,R}(x) = 1 \text{ for } |x| = R. \end{cases}$$

Here, the boundary radius R is chosen of order $N^{-\beta}$. That is, $F(x_i - x_j) \approx j_{N,R}(x_i - x_j)$ for $|x_i - x_j| = \mathcal{O}(N^{-\beta})$ and $F(x_i - x_j) = 1$ for $|x_i - x_j| \gg \mathcal{O}(N^{-\beta})$. Rescaling to coordinates

¹ One should however note that Ψ_t will not be close to a full product $\prod_{k=1}^N \varphi_t(x_k)$ in norm. For certain types of interactions, it has been shown rigorously that Ψ_t can be approximated by a quasifree state satisfying a Bogolubov-type dynamics, see [9], [53], [54] and [51] for precise statements.

$y = N^\beta x$, the zero energy scattering state satisfies

$$\left(-\Delta_y + \frac{1}{2} N^{-1} W(y) \right) j_{N,N^\beta R}(y) = 0. \quad (3.4)$$

Due to the factor N^{-1} in front of W , the zero energy scattering equation is almost constant, that is $j_{N,R}(x) \approx 1$, for all $|x| \leq R$. As a consequence, the microscopic structure F , induced by the zero energy scattering state, vanishes for any $\beta > 0$ and does not effect the dynamics of the reduced density matrix $\gamma_{\Psi_t}^{(1)}$. Assuming $\gamma_{\Psi_0}^{(1)} \approx |\varphi_0\rangle\langle\varphi_0|$, one may thus apply a law of large numbers argument and conclude that the interaction on each particle is then approximately given by its mean value

$$\int_{\mathbb{R}^2} d^2y N W_\beta(x-y) |\varphi_t|^2(y) \rightarrow \int_{\mathbb{R}^2} W(x) d^2x |\varphi_t|^2(x).$$

This yields to the correct coupling in the effective equation (3.3) in the case $U(x) = W_\beta(x)$. Let us now consider the case for which the dynamics of Ψ_t is generated by the Hamiltonian H_{V_N} . If one would guess the effective coupling of φ_t to be also given by its mean value w.r.t. the distribution $|\varphi_t|^2$, one would end up with the N -dependent equation $i\partial_t \varphi_t = (-\Delta + A_t) \varphi_t + N \int_{\mathbb{R}^2} d^2x V(x) |\varphi_t|^2 \varphi_t$. Note that the coupling constant of the self interaction differs from its correct value by a factor of $\mathcal{O}(N)$. As in the three dimensional Gross-Pitaevskii regime $\beta = 1$, it is now important to take the correlations explicitly into account. The scaling of the potential yields to $j_{N,R}(x) = j_{0,e^N R}(e^N x)$, which implies that the correlation function will influence the dynamics whenever two particles collide. The coupling parameter can then be inferred from the relation

$$\int_{\mathbb{R}^2} d^2x V_N(x) j_{N,R}(x) = \begin{cases} \frac{4\pi}{\ln(\frac{R}{ae^{-N}})} & \text{if } a > 0, \\ 0 & \text{if } a = 0, \end{cases}$$

where a denotes the scattering length of the potential $\frac{1}{2}V$. As mentioned, the logarithmic dependence of the integral above on a is special in two dimensions. Since $\frac{4\pi}{\ln(\frac{R}{ae^{-N}})} \approx \frac{4\pi}{N}$ holds for $a > 0$, the effective equation for φ_t will not depend on a anymore. Consequently, one obtains as an effective coupling

$$\int_{\mathbb{R}^2} d^2y N V_N(x-y) j_{N,R}(x-y) |\varphi_t|^2(y) \rightarrow \begin{cases} 4\pi |\varphi_t|^2(x) & \text{if } a > 0, \\ 0 & \text{if } a = 0. \end{cases}$$

We like to remark that it is easy to verify that, for any $s > 0$, the potential $V_{sN}(x) = e^{2Ns} V(e^{Ns} x)$ yields, for $a > 0$, to an effective coupling $4\pi/s$, resp. 0 in the case $a = 0$. For the sake of simplicity, we will not consider this slight generalization, although our proof is also valid in this case.

The rigorous derivation of effective evolution equations is well known in the literature, see e.g. [2, 4, 5, 7, 8, 9, 14, 17, 18, 19, 20, 25, 26, 30, 31, 32, 34, 49, 50, 51, 53, 54, 55, 59,

60, 61, 65] and references therein. For the two-dimensional case we consider, it has been proven, for $0 < \beta < 3/4$ and W nonnegative, that $\gamma_{\Psi_t}^{(1)}$ converges to $|\varphi_t\rangle\langle\varphi_t|$ as $N \rightarrow \infty$ [30]. Recently, the validity of the Bogoloubov approximation for the two-dimensional attractive bose gas was shown in [55] for $0 < \beta < 1$. We will discuss this result in more detail in Chapter 5.

Another approach which relates more closely to the experimental setup is to consider a three-dimensional gas of Bosons which is strongly confined in one spatial dimension. Then, one obtains an effective two dimensional system in the unconfined directions. We remark that in this dimensional reduction two limits appear, the length scale in the confined direction and the scaling of the interaction in the unconfined directions. Results in this direction can be found in [1] and [32], see also [31]. It is still an open problem to derive our dynamical result starting from a strongly confined three dimensional system. For known results regarding the ground state properties of dilute Bose gases, we refer to the monograph [41], which also summarizes the papers [39], [42] and [43].

Our proof is based on [60], where the emergence of the Gross-Pitaevskii equation was proven in three dimensions for $\beta = 1$. In particular, we adapt some crucial ideas which allow us to control the microscopic structure of Ψ_t .

We shall shortly discuss the physical relevance of the different scalings. For the exponential scaling $V_N(x) = e^{2N}V(e^N x)$, it is possible to rescale space- and time-coordinates in such a way that in the new coordinates the interaction is *not* N dependent. Choosing $y = e^N x$ and $\tau = e^{2N}t$ the Schrödinger equation reads

$$i \frac{d}{d\tau} \Psi_{e^{-2N}\tau} = \left(- \sum_{j=1}^N \Delta_{y_j} + \sum_{1 \leq j < k \leq N} V(y_j - y_k) + \sum_{j=1}^N A_{e^{-2N}\tau}(e^{-N}y_j) \right) \Psi_{e^{-2N}\tau}.$$

The latter equation thus corresponds to an extremely dilute gas of bosons with density $\sim e^{-2N}$. In order to observe a nontrivial dynamics, this condensate is then monitored over time scales of order $\tau \sim e^{2N}$. Since the trapping potential is adjusted according to the density of the gas in the experiment, the N dependence of $A_{e^{-2N}\tau}(e^{-N}\cdot)$ is reasonable.

3.2 Main result

We will consider initial wavefunctions Ψ_0 which are chosen such that the energy per particle is close to the effective Gross-Pitaevskii energy.

Definition 3.2.1 Define for $U \in \{W_\beta, V_N\}$ the energy functional $\mathcal{E}_U : H^2(\mathbb{R}^{2N}, \mathbb{C}) \rightarrow \mathbb{R}$

$$\mathcal{E}_U(\Psi) = N^{-1} \langle\langle \Psi, H_U \Psi \rangle\rangle.$$

Furthermore, define the Gross-Pitaevskii energy functional $\mathcal{E}_{b_U}^{GP} : H^1(\mathbb{R}^2, \mathbb{C}) \rightarrow \mathbb{R}$

$$\mathcal{E}_{b_U}^{GP}(\varphi) = \langle \nabla \varphi, \nabla \varphi \rangle + \langle \varphi, (A_t + \frac{1}{2}b_U|\varphi|^2)\varphi \rangle = \langle \varphi, (h_{b_U}^{GP} - \frac{1}{2}b_U|\varphi|^2)\varphi \rangle. \quad (3.5)$$

Note that both $\mathcal{E}_U(\Psi)$ and $\mathcal{E}_{b_U}^{GP}(\varphi)$ depend on t , due to the time varying external potential A_t . For the sake of readability, we will not indicate this time dependence explicitly. Next, we will specify the class of potentials V we will consider.

Definition 3.2.2 Let $B_r(x) = \{z \in \mathbb{R}^2 \mid |x - z| < r\}$ and divide \mathbb{R}^2 into rectangles C_n , $n \in \mathbb{Z}$ of side length $b_1/\sqrt{2}$; that is $\mathbb{R}^2 = \bigcup_{n=-\infty}^{\infty} C_n$. Furthermore, assume that $\overset{\circ}{C}_n \cap \overset{\circ}{C}_m = \emptyset$ for $m \neq n$. Define

$$n(b_1, b_2) = \max_{x \in \mathbb{R}^2} \#\{n : C_n \cap B_{b_2}(x) \neq \emptyset\}.$$

Thus, $n(b_1, b_2)$ gives the maximal number of rectangles with side length $b_1/\sqrt{2}$ one needs to cover a sphere with radius b_2 .

Assumption 3.2.3 Let $V \in L_c^\infty(\mathbb{R}^2, \mathbb{R})$ spherically symmetric and let $V(x) = V^+(x) - V^-(x)$, where $V^+, V^- \in L_c^\infty(\mathbb{R}^2, \mathbb{R})$ are spherically symmetric, such that $V^+(x), V^-(x) \geq 0$ and the supports of V^+ and V^- are disjoint. Assume that

- (a) Let $R > r_2 > 0$ and assume $\text{supp}(V^+) \in B_{r_2}(0)$, as well as $\text{supp}(V^-) \in B_R(0) \setminus B_{r_2}(0)$.
- (b) There exists $\lambda^+ > 0$ and $r_1 > 0$, such that $V^+(x) \geq \lambda^+$ for all $x \in B_{r_1}(0)$.
- (c) Define $\lambda^- = \|V^-\|_\infty$, as well as $n_1 = n(r_1, R)$ and $n_2 = n(r_1, 3R)$. Define, for $0 < \epsilon < 1$,

$$\mathcal{E}_R(\varphi) = \int_{B_R(0)} \left(|\nabla_x \varphi(x)|^2 + \frac{1}{1-\epsilon} n_1 (2V^+(x) - 4V^-(x)) |\varphi(x)|^2 \right) d^2x. \quad (3.6)$$

We then assume that for some $0 < \epsilon < 1$

$$\inf_{\varphi \in C^1(\mathbb{R}^2, \mathbb{C}), \varphi(R)=1} (\mathcal{E}_R(\varphi)) \geq 0, \quad (3.7)$$

$$\lambda^+ > 8n_2\lambda^-. \quad (3.8)$$

Remark 3.2.4 Assumption 3.2.3 is discussed in detail in Chapter 4. There, we also provide some estimates necessary to prove the next theorem.

We now state our main Theorem:

Theorem 3.2.5 Let $\Psi_0 \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap H^2(\mathbb{R}^{2N}, \mathbb{C})$ with $\|\Psi_0\| = 1$. Let $\varphi_0 \in L^2(\mathbb{R}^2, \mathbb{C})$ with $\|\varphi_0\| = 1$ and assume $\lim_{N \rightarrow \infty} \gamma_{\Psi_0}^{(1)} = |\varphi_0\rangle\langle\varphi_0|$ in trace norm. Let the external potential A_t , which appears in the Hamiltonian (3.2), satisfy $A_t \in C^1(\mathbb{R}, L^\infty(\mathbb{R}^2, \mathbb{R}))$.

(a) For any $\beta > 0$, let W_β be given by $W_\beta(x) = N^{-1+2\beta}W(N^\beta x)$, for $W \in L_c^\infty(\mathbb{R}^2, \mathbb{R})$ and W spherically symmetric. Assume $-(1-\epsilon)\Delta + \frac{1}{2}W \geq 0$ on $L^2(\mathbb{R}^2, \mathbb{C})$ for some $\epsilon > 0$. Let Ψ_t the unique solution to $i\partial_t\Psi_t = H_{W_\beta}\Psi_t$ with initial datum Ψ_0 . Let φ_t the unique solution to $i\partial_t\varphi_t = h_{\int_{\mathbb{R}^2} W(x)d^2x}^{GP}\varphi_t$ with initial datum φ_0 and assume that $\varphi_t \in H^3(\mathbb{R}^2, \mathbb{C})$. Let $\lim_{N \rightarrow \infty} (\mathcal{E}_{W_\beta}(\Psi_0) - \mathcal{E}_{b_W}^{GP}(\varphi_0)) = 0$. Then, for any $\beta > 0$ and for any $t > 0$

$$\lim_{N \rightarrow \infty} \gamma_{\Psi_t}^{(1)} = |\varphi_t\rangle\langle\varphi_t| \quad (3.9)$$

in trace norm.

(b) Let V_N be given by $V_N(x) = e^{2N}V(e^N x)$ and let V satisfy Assumption 3.2.3. Let Ψ_t the unique solution to $i\partial_t\Psi_t = H_{V_N}\Psi_t$ with initial datum Ψ_0 . Let either condition (I) or condition (II) fulfilled, where

(I) Let the scattering length a of $\frac{1}{2}V$ fulfill $a > 0$. Let φ_t the unique solution to $i\partial_t\varphi_t = h_{4\pi}^{GP}\varphi_t$ with initial datum φ_0 assume that $\varphi_t \in H^3(\mathbb{R}^2, \mathbb{C})$. Let $\lim_{N \rightarrow \infty} (\mathcal{E}_{V_N}(\Psi_0) - \mathcal{E}_{4\pi}^{GP}(\varphi_0)) = 0$.

(II) Let the scattering length a of $\frac{1}{2}V$ fulfill $a = 0$. Let φ_t the unique solution to $i\partial_t\varphi_t = (-\Delta + A_t)\varphi_t$ with initial datum $\varphi_0 \in H^3(\mathbb{R}^2, \mathbb{C})$.

$$\text{Let } \lim_{N \rightarrow \infty} (\mathcal{E}_{V_N}(\Psi_0) - \mathcal{E}_0^{GP}(\varphi_0)) = 0.$$

Then, for any $t > 0$

$$\lim_{N \rightarrow \infty} \gamma_{\Psi_t}^{(1)} = |\varphi_t\rangle\langle\varphi_t| \quad (3.10)$$

in trace norm.

Remark:

(a) We expect that for regular enough external potentials A_t , the regularity assumption $\varphi_t \in H^3(\mathbb{R}^2, \mathbb{C})$ to follow from regularity assumptions on the initial datum φ_0 . In particular, if $\varphi_0 \in \Sigma^3(\mathbb{R}^2, \mathbb{C}) = \{f \in L^2(\mathbb{R}^2, \mathbb{C}) \mid \sum_{\alpha+\beta \leq 3} \|\langle x^\alpha \partial_x^\beta f \rangle\| < \infty\}$ holds, the bound $\|\varphi_t\|_{H^3} < \infty$ has been proven for external potentials which are at most quadratic in space, see [11] and Lemma 3.6.1. In particular, for $\varphi_0 \in \Sigma^3(\mathbb{R}^2, \mathbb{C})$, the bound $\|\varphi_t\|_{H^3} \leq C$ holds if the external potential is not present, i.e. $A_t = 0$.

(b) For nonnegative potentials V , it has been shown that in the limit $N \rightarrow \infty$ the energy-difference $\mathcal{E}_{V_N}(\Psi^{gs}) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi^{gs}) \rightarrow 0$, where Ψ^{gs} is the ground state of a trapped Bose gas and φ^{gs} the ground state of the respective Gross-Pitaevskii energy functional, see [43], [42].

(c) It is well known that in the scattering length of a two-dimensional Bose gas is non-negative (see e.g. Appendix C of [41]). Thus, the scattering length of $\frac{1}{2}V$ is either zero or positive.

- (d) In our proof we will give explicit error estimates in terms of the particle number N . We shall show that the rate of convergence is of order $N^{-\delta}$ for some $\delta > 0$, assuming that also initially $\gamma_{\Psi_0}^{(1)} \rightarrow |\varphi_0\rangle\langle\varphi_0|$ converges in trace norm with rate of at least $N^{-\delta}$.
- (e) One can relax the conditions on the initial condition and only require $\Psi_0 \in L_s^2(\mathbb{R}^{2N}, \mathbb{C})$ using a standard density argument.

3.2.1 Organization of the proof

Our proof is based on [60], which covers the three-dimensional counterpart of our system. The proof is organized as follows:

- (a) First, we will introduce in Section 3.3 the zero energy scattering state. We explain how the effective coupling parameter b_{V_N} can be inferred from the microscopic structure.
- (b) In Section 3.4.1 we consider the potential W_β and define some convenient counting measure which allows us to perform a Grönwall type estimate for all $\beta > 0$. We will explain in detail how one arrives at this Grönwall estimate.
- (c) For the most difficult scaling given by the potential V_N , it is crucial to take the interaction-induced correlations between the particles into account. In Section 3.4.2, we will adapt the counting measure to account for this correlation structure.
- (d) In Section 3.5, we provide the necessary estimates for the Grönwall estimates.
- (e) In Section 3.6, we will comment on the solution theory of φ_t .

Notation 3.2.6 *In the following, we will denote by $\mathcal{K}(\varphi_t, A_t)$ a generic polynomial with finite degree in $\|\varphi_t\|_\infty, \|\nabla\varphi_t\|_\infty, \|\nabla\varphi_t\|, \|\Delta\varphi_t\|, \|A_t\|_\infty, \int_0^t ds \|\dot{A}_s\|_\infty$ and $\|\dot{A}_t\|_\infty$.*

Remark 3.2.7 *By the Sobolev embedding Theorem, it is possible to bound*

$$\|\varphi_t\|_\infty + \|\nabla\varphi_t\|_\infty + \|\nabla\varphi_t\| + \|\Delta\varphi_t\| \leq C \|\varphi_t\|_{H^3(\mathbb{R}^2, \mathbb{C})},$$

Under the assumptions of Theorem 3.2.5, it therefore follows that there exists a constant C_t , depending on time, such that $\mathcal{K}(\varphi_t, A_t) \leq C_t$ holds². We will comment on the solution theory of φ_t in Section 3.6.

Also note that for a generic constant C the inequality $C \leq \mathcal{K}(\varphi_t, A_t)$ holds. The exact form of $\mathcal{K}(\varphi_t, A_t)$ which appears in the final bounds could be reconstructed in principle, collecting all contributions from the different estimates.

² Actually, $\varphi_t \in H^{2+\epsilon}(\mathbb{R}^2, \mathbb{C})$ for some $\epsilon > 0$ would suffice for our estimates.

3.3 Microscopic structure in 2 dimensions

3.3.1 The scattering state

In this section, we analyze the microscopic structure which is induced by V_N . In particular, we explain why the dynamical properties of the system are determined by the low energy scattering regime.

Definition 3.3.1 *Let $V \in L_c^\infty(\mathbb{R}^2, \mathbb{R})$, V spherically symmetric and let V_N be given by $V_N(x) = e^{2N}V(e^N x)$. In the following, let R denote the radius of the support of V . For any $\mathcal{R} \geq e^{-N}R$, we define the zero energy scattering state $j_{N,\mathcal{R}}$ by*

$$\begin{cases} \left(-\Delta_x + \frac{1}{2}e^{2N}V(e^N x) \right) j_{N,\mathcal{R}}(x) = 0, \\ j_{N,\mathcal{R}}(x) = 1 \text{ for } |x| = \mathcal{R}. \end{cases} \quad (3.11)$$

One may think of \mathcal{R} as the mean interparticle distance of the condensate, i.e. $\mathcal{R} = \mathcal{O}(N^{-1/2})$. However, one is quite free in choosing \mathcal{R} , since the dependence of $j_{N,\mathcal{R}}$ on \mathcal{R} is only logarithmic (see below).

Next, we want to recall some important properties of the scattering state $j_{N,\mathcal{R}}$, see also Appendix C of [41].

Lemma 3.3.2 *Let $V \in L_c^\infty(\mathbb{R}^2, \mathbb{C})$ spherically symmetric and assume V satisfies Assumption 3.2.3. Define $I_{\mathcal{R}} = \int_{\mathbb{R}^2} d^2x V_N(x) j_{N,\mathcal{R}}(x)$. For the scattering state defined previously the following relations hold:*

(a) *There exists a nonnegative number a , called scattering length of the potential $\frac{1}{2}V$, such that*

$$I_{\mathcal{R}} = \frac{4\pi}{\ln\left(\frac{e^N \mathcal{R}}{a}\right)}$$

(in the case $a = 0$ we have $I_{\mathcal{R}} = 0$). The scattering length a does not depend on \mathcal{R} and fulfills $a \leq R$. Furthermore, $I_{\mathcal{R}} \geq 0$ holds.

(b) *$j_{N,\mathcal{R}}$ is a nonnegative nondecreasing function which is spherically symmetric in $|x|$. For $|x| \geq e^{-N}R$, $j_{N,\mathcal{R}}$ is given by*

$$j_{N,\mathcal{R}}(x) = 1 + \frac{1}{\ln\left(\frac{e^N \mathcal{R}}{a}\right)} \ln\left(\frac{|x|}{\mathcal{R}}\right).$$

Proof:

(a)+(b) Rescaling $x \rightarrow e^N x = y$, we obtain, setting $\tilde{R} = e^N \mathcal{R}$ and $s_{\tilde{R}}(y) = j_{0,e^N \mathcal{R}}(y)$, the unscaled scattering equation

$$\begin{cases} (-\Delta_y + \frac{1}{2}V(y)) s_{\tilde{R}}(y) = 0, \\ s_{\tilde{R}}(y) = 1 \text{ for } |y| = \tilde{R}. \end{cases} \quad (3.12)$$

Under the Assumption 3.2.3 on V , we have $-\Delta + \frac{1}{2}V \geq 0$. Therefore, one can define the scattering state $s_{\tilde{R}}$ by a variational principle. Theorem C.1 in [41] then implies that $s_{\tilde{R}}$ is a nonnegative, spherically symmetric function in $|x|$. It is then easy to verify that for $R \leq |x|$ there exists a number $A \in \mathbb{R}$ such that

$$s_{\tilde{R}}(x) = 1 + \frac{A}{4\pi} \ln \left(\frac{|x|}{\tilde{R}} \right). \quad (3.13)$$

Next, we show that $A = \int_{\mathbb{R}^2} d^2x V(x) s_{\tilde{R}}(x)$. This can be seen by noting that, for $r > R$,

$$\begin{aligned} \int_{\mathbb{R}^2} d^2x V(x) s_{\tilde{R}}(x) &= 2 \int_{B_r(0)} d^2x \Delta s_{\tilde{R}}(x) = 2 \int_{\partial B_r(0)} \nabla s_{\tilde{R}}(x) \cdot ds \\ &= \frac{A}{2\pi} \int_{\partial B_r(0)} \nabla \ln(|x|) \cdot ds = \frac{A}{2\pi} \int_0^{2\pi} \frac{1}{r} r d\varphi \\ &= A. \end{aligned}$$

By Theorem C.1 in [41], there exists a number $a \geq 0$, not depending on \tilde{R} , such that for all $|x| \geq R$

$$s_{\tilde{R}}(x) = \frac{\ln(|x|/a)}{\ln(\tilde{R}/a)}.$$

Comparing this with (3.13), we obtain

$$\int_{\mathbb{R}^2} V(x) s_{\tilde{R}}(x) dx^2 = \frac{4\pi}{\ln\left(\frac{\tilde{R}}{a}\right)}.$$

Since $s_{\tilde{R}}$ is nonnegative, it furthermore follows that $a \leq R$. This directly implies $A \geq 0$. By scaling, we obtain

$$I_{\tilde{R}} = \int_{\mathbb{R}^2} V_N(x) j_{N,\mathcal{R}}(x) dx^2 = \int_{\mathbb{R}^2} V(x) s_{\tilde{R}}(x) dx^2 = \frac{4\pi}{\ln\left(\frac{e^N \mathcal{R}}{a}\right)}.$$

It is left to show that $s_{\tilde{R}}$ is monotone nondecreasing in $|x|$. Define for $r \in \mathbb{R}$

$$\tilde{I}_r = \int_{B_r(0)} V(x) s_{\tilde{R}}(x) dx^2$$

Since V is supported on $B_R(0)$, the identity $I_{\mathcal{R}} = \tilde{I}_{\mathcal{R}}$ holds. Let $t(|x|) = s_{\tilde{R}}(x)$. By Gauß-theorem and the scattering equation (3.11), it then follows for $r > 0$

$$\frac{d}{dr}t(r) = \frac{\tilde{I}_r}{4\pi r}.$$

Since $t(r) \geq 0$ holds for all $r \geq 0$, it follows $\tilde{I}_r > 0$ for all $r \in]0, r_2[$, with r_2 being defined as in Assumption 3.2.3. If it were now that j is not monotone nondecreasing, there must exist a $\tilde{r} \geq r_2$, such that $\tilde{I}_{\tilde{r}} < 0$. $V(x) \leq 0$ and $t(r) \geq 0$ for all $|x| \in]r_2, \mathcal{R}[$ then imply $\tilde{I}_r \leq \tilde{I}_{\tilde{r}}$ for all $r \geq \tilde{r}$. This, however, contradicts $I_{\mathcal{R}} = \tilde{I}_{\mathcal{R}} \geq 0$. Thus, it follows that $s_{\tilde{R}}$ is monotone nondecreasing.

□

Remark 3.3.3 Note that for $|x| \gg e^{-N}R$ and N large enough, the scattering state $j_{N,\mathcal{R}}(x) \approx 1$ is almost constant, regardless of the specific choice of the normalization radius \mathcal{R} . In other words, the scattering state essentially only varies on length scales which are determined by the potential V_N , i.e. on length scales of order $\mathcal{O}(e^{-N})$.

Assuming that the energy per particle $\mathcal{E}_{V_N}(\Psi)$ is of order one, the wave function Ψ will have a microscopic structure near the interactions V_N , given by $j_{N,\mathcal{R}}$. For a positive scattering length $a > 0$, the interaction among two particles is then determined by $\frac{4\pi}{N + \ln(\frac{\mathcal{R}}{a})} \approx \frac{4\pi}{N}$. Keeping in mind that each particle interacts with all other $N - 1$ particles, we obtain the effective Gross-Pitaevskii equation, for $\varphi_t \in H^2(\mathbb{R}^2, \mathbb{C})$

$$i\partial_t \varphi_t(x) = (-\Delta + A_t + 4\pi|\varphi_t(x)|^2)\varphi_t(x)$$

If $a = 0$, φ_t obeys the one-particle Schrödinger equation with the external field A_t . Thus, choosing $V_N(x) = e^{2N}V(e^N x)$ leads in our setting to an effective one-particle equation which is determined by the low energy scattering behavior of the particles. We remark that, for any $s > 0$, the potential $e^{2Ns}V(e^{Ns}x)$ yields to the coupling $4\pi/s$ in the case $a > 0$, respectively 0 for $a = 0$.

3.3.2 Properties of the scattering state

Note that the potential V_N is strongly peaked within an exponentially small region. In order to control the short scale structure of Ψ_t , we define, with a slight abuse of notation, a potential M_β with softer scaling behavior in such a way that the potential $\frac{1}{2}(V_N - M_\beta)$ has scattering length zero. This allows us to “replace” V_N by M_β , which has better scaling behavior and is easier to control. In particular, $\|M_\beta\| \leq CN^{-1+\beta}$ can be controlled for β sufficiently small, while $\|V_N\| = \mathcal{O}(e^N)$ cannot be bounded by any finite polynomial in N . The potential M_β is *not* of the exact scaling $N^{-1+2\beta}M(N^\beta x)$. However, it is in the set \mathcal{V}_β , which we will define now.

Definition 3.3.4 For any $\beta > 0$, we define the set of potentials \mathcal{V}_β as

$$\mathcal{V}_\beta = \left\{ U \in L^2(\mathbb{R}^2, \mathbb{R}) \mid \begin{array}{l} \|U\|_1 \leq CN^{-1}, \|U\| \leq CN^{-1+\beta}, \\ \|U\|_\infty \leq CN^{-1+2\beta}, U(x) = 0 \forall |x| \geq CN^{-\beta}, U \text{ is spherically symmetric} \end{array} \right\}.$$

Note that $N^{-1+2\beta}W(N^\beta x) \in \mathcal{V}_\beta$ holds, if W is spherically symmetric and compactly supported.

All relevant estimates in this chapter are formulated for $W_\beta \in \mathcal{V}_\beta$.

Definition 3.3.5 Let $V \in L_c^\infty(\mathbb{R}^2, \mathbb{C})$ fulfill Assumption 3.2.3. For any $\beta > 0$ and any $R_\beta \geq N^{-\beta}$ we define the potential M_β via

$$M_\beta(x) = \begin{cases} 4\pi N^{-1+2\beta} & \text{if } N^{-\beta} < |x| \leq R_\beta, \\ 0 & \text{else.} \end{cases} \quad (3.14)$$

Furthermore, we define the zero energy state f_β of the potential $\frac{1}{2}(V_N(x) - M_\beta(x))$, that is

$$\begin{cases} \left(-\Delta_x + \frac{1}{2}(V_N(x) - M_\beta(x)) \right) f_\beta(x) = 0 \\ f_\beta(x) = 1 \text{ for } |x| = R_\beta \end{cases}. \quad (3.15)$$

Note that M_β and f_β depend on R_β . We choose R_β such that the scattering length of the potential $\frac{1}{2}(V_N - M_\beta(x))$ is zero. This is equivalent to the condition $\int_{\mathbb{R}^2} d^2x (V_N(x) - M_\beta(x)) f_\beta(x) = 0$.

Lemma 3.3.6 For the scattering state f_β , defined by Equation (3.15), the following relations hold:

(a) There exists a minimal value $R_\beta < \infty$ such that $\int_{\mathbb{R}^2} d^2x (V_N(x) - M_\beta(x)) f_\beta(x) = 0$.

For the rest of the chapter we assume that R_β is chosen such that (a) holds.

(b) There exists $K_\beta \in \mathbb{R}$, $K_\beta > 0$ such that $K_\beta f_\beta(x) = j_{N,R_\beta}(x) \forall |x| \leq N^{-\beta}$.

(c) For N sufficiently large the supports of V_N and M_β do not overlap.

(d) f_β is a nonnegative function in $|x|$ which is monotone nondecreasing for all $N^{-\beta} \leq |x| < R_\beta$.

(e)

$$f_\beta(x) = 1 \text{ for } |x| \geq R_\beta. \quad (3.16)$$

(f)

$$1 \geq K_\beta \geq 1 + \frac{1}{N + \ln\left(\frac{R_\beta}{a}\right)} \ln\left(\frac{N^{-\beta}}{R_\beta}\right). \quad (3.17)$$

(g) $R_\beta \leq CN^{-\beta}$.

For any fixed $0 < \beta$, N sufficiently large such that V_N and M_β do not overlap, we obtain

(h)

$$\left| N \int_{\mathbb{R}^2} d^2x V_N(x) f_\beta(x) - b_{V_N} \right| = |N \|M_\beta f_\beta\|_1 - b_{V_N}| \leq C \frac{\ln(N)}{N}.$$

(i) Define

$$g_\beta(x) = 1 - f_\beta(x).$$

Then,

$$\|g_\beta\|_1 \leq CN^{-2\beta}, \quad \|g_\beta\| \leq CN^{-\beta}, \quad \|g_\beta\|_\infty \leq C.$$

(j)

$$|N \|M_\beta\|_1 - b_{V_N}| \leq C \frac{\ln(N)}{N}.$$

(k)

$$M_\beta \in \mathcal{V}_\beta, M_\beta f_\beta \in \mathcal{V}_\beta, M_\beta f_\beta \geq 0.$$

Remark: If the scattering length a of the potential $\frac{1}{2}V$ is zero, it is not necessary to introduce the potential M_β . For a unified presentation, we have not distinguished the cases $a > 0$ and $a = 0$ in this chapter. In the latter case $a = 0$, we can choose $R_\beta = N^{-\beta}$, $M_\beta = 0$, $f_\beta(x) = j_{N,\mathcal{R}}$ and $K_\beta = 1$. Part (j) and (k) are then trivially true. Furthermore, all other parts follow from Lemma 3.3.2. We may thus assume $a > 0$, $R_\beta > N^{-\beta}$ and $b_{V_N} = 4\pi$ in the following proof.

Proof:

- (a) In the following, we will sometimes denote, with a slight abuse of notation, $f_\beta(x) = f_\beta(r)$ and $j_{N,\mathcal{R}}(x) = j_{N,\mathcal{R}}(r)$ for $r = |x|$ (for this, recall that f_β and $j_{N,\mathcal{R}}$ are radially symmetric). We further denote by $f'_\beta(r)$ the derivative of f_β with respect to the radial coordinate r .

We first show by contradiction that there exists a $x_0 \in \mathbb{R}^2$, $|x_0| \leq N^{-\beta}$, such that $f_\beta(x_0) \neq 0$. For this, assume that $f_\beta(x) = 0$ for all $|x| \leq N^{-\beta}$. Since f_β is continuous, there exists a maximal value $r_0 \geq N^{-\beta}$ such that the scattering equation (3.15) is equivalent to

$$\begin{cases} (-\Delta_x - \frac{1}{2}M_\beta(x))f_\beta(x) = 0, \\ f_\beta(x) = 1 \text{ for } |x| = R_\beta, \\ f_\beta(x) = 0 \text{ for } |x| \leq r_0. \end{cases} \quad (3.18)$$

Using (3.15) and Gauss'-theorem, we further obtain

$$f'_{\beta_1,1}(r) = \frac{1}{4\pi r} \int_{B_r(0)} d^2x (V_N(x) - M_\beta(x)) f_\beta(x). \quad (3.19)$$

(3.18) and (3.19) then imply for $r > r_0$

$$\begin{aligned} |f'_\beta(r)| &= \frac{1}{4\pi r} \left| \int_{B_r(0)} d^2x M_\beta(x) f_\beta(x) \right| = \frac{2\pi N^{-1+2\beta}}{r} \left| \int_{r_0}^r dr' r' f_\beta(r') \right| \\ &\leq \frac{2\pi N^{-1+2\beta}}{r} \left| \int_{r_0}^r dr' r' (r' - r_0) \sup_{r_0 \leq s \leq r} |f'_\beta(s)| \right|. \end{aligned}$$

Taking the supreme over the interval $[r_0, r]$, the inequality above then implies that there exists a constant $C(r, r_0) \neq 0$, $\lim_{r \rightarrow r_0} C(r, r_0) = 0$ such that $\sup_{r_0 \leq s \leq r} |f'_\beta(s)| \leq C(r, r_0) N^{-1+3\beta_1} \sup_{r_0 \leq s \leq r} |f'_\beta(s)|$. Thus, for r close enough to r_0 , the inequality above can only hold if $f'_\beta(s) = 0$ for $s \in [r_0, r]$, yielding a contradiction to the choice of r_0 . Consequently, there exists a $x_0 \in \mathbb{R}^2$, $|x_0| \leq N^{-\beta}$, such that $f_\beta(x_0) \neq 0$. We can thus define

$$h(x) = f_\beta(x) \frac{j_{N,\mathcal{R}}(x_0)}{f_\beta(x_0)}$$

on the compact set $\overline{B_{x_0}(0)}$. One easily sees that $h(x) = j_{N,\mathcal{R}}(x)$ on $\partial \overline{B_{x_0}(0)}$ and satisfies the zero energy scattering equation (3.11) for $x \in \overline{B_{N^{-\beta}}(0)}$. Note that the scattering equations (3.11) and (3.15) have a unique solution on any compact set. It then follows that $h(x) = j_{N,\mathcal{R}}(x) \forall x \in \overline{B_{N^{-\beta}}(0)}$. Since $j_{N,\mathcal{R}}(N^{-\beta}) \neq 0$, we then obtain $f_\beta(N^{-\beta}) \neq 0$. Applying Lemma 3.3.2, it then follows that either f_β or $-f_\beta$ is a nonnegative, monotone nondecreasing function in $|x|$ for all $|x| \leq N^{-\beta}$.

Recall that W_β and hence $f_\beta(x)$ depend on $R_\beta \in [N^{-\beta}, \infty[$. For conceptual clarity, we denote $W_\beta^{(R_\beta)}(x) = W_\beta(x)$ and $f_\beta^{(R_\beta)}(x) = f_\beta(x)$ for the rest of the proof of part (a). For β fixed, consider the function

$$s : [N^{-\beta}, \infty[\rightarrow \mathbb{R}, \quad (3.20)$$

$$R_\beta \mapsto \int_{B_{R_\beta}(0)} d^2x (V_N(x) - W_\beta^{(R_\beta)}(x)) f_\beta^{(R_\beta)}(x). \quad (3.21)$$

We show by contradiction that the function s has at least one zero. Assume $s \neq 0$ were to hold. We can assume w.l.o.g. $s > 0$. It then follows from Gauss'-theorem that $f_\beta'(R_\beta) > 0$ for all $R_\beta \geq N^{-\beta}$. By uniqueness of the solution of the scattering equation (3.15), for $\tilde{R}_\beta < R_\beta$ there exists a constant $K_{\tilde{R}_\beta, R_\beta} \neq 0$, such that for all $|x| \leq \tilde{R}_\beta$ we have $f_\beta^{(\tilde{R}_\beta)}(x) = K_{\tilde{R}_\beta, R_\beta} f_\beta^{(R_\beta)}(x)$. Since $f_\beta^{(R_\beta)}$ and s are continuous, we can further conclude $K_{\tilde{R}_\beta, R_\beta} > 0$. From $s \neq 0$, it then follows that, for all $r \in [N^{-\beta}, \infty[$ and for all $R_\beta \in [N^{-\beta}, \infty[$, $f_\beta^{(R_\beta)}(r) \neq 0$. Thus, for all $r \in [N^{-\beta}, \infty[$ and for all $R_\beta \in [N^{-\beta_1}, \infty[$, the function $f_\beta^{(R_\beta)}(r)$ doesn't change sign. From Lemma 3.3.2, the assumption $s(N^{-\beta}) > 0$ and $K_{\tilde{R}_\beta, R_\beta} > 0$, we obtain, for all $r \in [0, N^{-\beta}]$ and for all $R_\beta \in [N^{-\beta}, \infty[$, that $f_\beta^{(R_\beta)}(r) \geq 0$ holds. This, however, implies $\lim_{R_\beta \rightarrow \infty} s(R_\beta) = -\infty$ yielding to a contradiction. By continuity of s , there exists thus a minimal value $R_\beta \geq N^{-\beta}$ such that $s(R_\beta) = 0$.

Remark 3.3.7 As mentioned, we will from now on fix $R_\beta \in [N^{-\beta}, \infty[$ as the minimal value such that $s(R_\beta) = 0$. Furthermore, we may assume $a > 0$ and $R_\beta > N^{-\beta}$ in the following. For $a = 0$, we can choose $R_\beta = N^{-\beta}$, such that $f_\beta(x) = j_{N, R_\beta}(x)$.

(b) Since $f_\beta(N^{-\beta}) \neq 0$, it follows that

$$K_\beta = \frac{j_{N, R_\beta}(N^{-\beta})}{f_\beta(N^{-\beta})}. \quad (3.22)$$

Next, we show that the constant K_β is positive. Since $j_{N, R_\beta}(N^{-\beta})$ is positive, it follows from Eq. (3.22) that K_β and $f_\beta(N^{-\beta})$ have equal sign. By (a), the sign of f_β is constant for $|x| \leq R_\beta$. Furthermore, from Gauss-theorem and the scattering equation (3.15) we have

$$f_\beta'(r) = \frac{1}{4\pi r K_\beta} \int_{B_r(0)} d^2 x V_N(x) j_{N, R_\beta}(x) \quad (3.23)$$

for all $r \leq N^{-\beta}$. By Lemma 3.3.2, $\int_{\mathbb{R}^2} d^2 x V_N(x) j_{N, R_\beta}(x) > 0$ holds (note that we assume $a > 0$), which implies

$$\operatorname{sgn}(f_\beta'(N^{-\beta})) = \operatorname{sgn}(K_\beta). \quad (3.24)$$

Recall that R_β is the smallest value such that $f_\beta'(R_\beta) = 0$. If it were now that K_β is negative, we could conclude from (3.22) and (3.24) that $f_\beta'(N^{-\beta}) < 0$ and $f_\beta(N^{-\beta}) < 0$. Since R_β is by definition the smallest value where $f_\beta'(R_\beta) = 0$ holds, we were able to conclude from the continuity of the derivative that $f_\beta'(r) < 0$ for all $r < R_\beta$ and hence $f_\beta(R_\beta) < 0$. However, this were in contradiction to the boundary condition of the zero energy scattering state (see (3.15)) and thus $K_\beta > 0$ follows.

(c) This directly follows from $e^{-N} < CN^{-\beta}$ for N sufficiently large.

(d) From the proof of property (b), we see that f_β and its derivative is positive at $N^{-\beta}$. From (3.19), we obtain $f'_\beta(r) = 0$ for all $r > R_\beta$. Due to continuity, $f'_\beta(r) > 0$ for all $N^{-\beta} \leq r < R_\beta$. Since f_β is continuous, positive at $N^{-\beta}$, and its derivative is a nonnegative function, it follows that f_β is a nonnegative function in $|x|$ which is monotone nondecreasing for all $N^{-\beta} \leq |x| < R_\beta$.

(e) By definition of R_β , it follows that $\tilde{I} = \int_{\mathbb{R}^2} d^2x (V_N(x) - W_\beta(x)) f_\beta(x) = 0$. Therefore, for all $|x| \geq R_\beta$, f_β solves $-\Delta f_\beta(x) = 0$, which has the solution

$$f_\beta(x) = 1 + \frac{\tilde{I}}{4\pi} \ln\left(\frac{|x|}{R_\beta}\right) = 1.$$

(f) Since f_β is a positive monotone nondecreasing function in $|x|$, for $|x| \geq N^{-\beta}$, we obtain

$$1 \geq f_\beta(N^{-\beta}) = j_{N,R_\beta}(N^{-\beta})/K_\beta = \left(1 + \frac{1}{N + \ln\left(\frac{R_\beta}{a}\right)} \ln\left(\frac{N^{-\beta}}{R_\beta}\right)\right) / K_\beta.$$

We obtain the lower bound

$$K_\beta \geq 1 + \frac{1}{N + \ln\left(\frac{R_\beta}{a}\right)} \ln\left(\frac{N^{-\beta}}{R_\beta}\right).$$

For the upper bound we first prove that $f_\beta(x) \geq j_{N,R_\beta}(x)$ holds for all $|x| \leq R_\beta$. Define $m(x) = j_{N,R_\beta}(x) - f_\beta(x)$. Using the scattering equations (3.13) and (3.15) we obtain

$$\begin{cases} \Delta_x m(x) = \frac{1}{2} V_N(x) m(x) + \frac{1}{2} W_\beta(x) f_\beta(x), \\ m(R_\beta) = 0. \end{cases}$$

Let $D = e^{-N} R$, where, as above, R denotes the radius of the support of the potential V . Since $W_\beta(x) f_\beta(x) \geq 0$, we obtain that $\Delta_x m(x) \geq 0$ for $D \leq |x| \leq R_\beta$. That is, $m(x)$ is subharmonic for $D < |x| < R_\beta$. Using the maximum principle, we obtain, using that $m(x)$ is spherically symmetric

$$\max_{D \leq |x| \leq R_\beta} (m(x)) = \max_{|x| \in \{D, R_\beta\}} (m(x)). \quad (3.25)$$

If it were now that $\max_{|x| \in \{D, R_\beta\}} (m(x)) = m(D) \geq m(R_\beta) = 0$, we could conclude that $m(x) \geq 0$ for all $D \leq |x| \leq R_\beta$. Assume that $m(D) > 0$ (otherwise we can conclude $j_{N,R_\beta}(N^{-\beta}) = f_\beta(N^{-\beta})$ which implies $K_\beta = 1$). Note that $m(x)$ then solves

$$\begin{cases} -\Delta_x m(x) + \frac{1}{2} V_N(x) m(x) = 0 \text{ for } |x| \leq N^{-\beta}, \\ m(D) > 0. \end{cases}$$

By Theorem C.1 in [41] (note that we assume $a > 0$), m is strictly increasing for $D \leq |x| \leq N^{-\beta}$. This, however, contradicts $\max_{|x| \in \{D, R_\beta\}}(m(x)) = m(D)$.

Therefore, we can conclude in (3.25) that $\max_{|x| \in \{D, R_\beta\}}(m(x)) = m(R_\beta) = 0$ holds. Then, it follows that $f_\beta(x) - j_{N, R_\beta}(x) \geq 0$ for all $D \leq |x| \leq R_\beta$. Using the zero energy scattering equation $-\Delta(f_\beta(x) - j_{N, R_\beta}(x)) + \frac{1}{2}V_N(x)(f_\beta(x) - j_{N, R_\beta}(x)) = 0$ for $|x| \leq N^{-\beta}$, we can, together with $f_\beta(N^{-\beta}) - j_{N, R_\beta}(N^{-\beta}) \geq 0$, conclude that $f_\beta(x) - j_{N, R_\beta}(x) \geq 0$ for all $|x| \leq R_\beta$.

As a consequence, we obtain the desired bound $K_\beta = \frac{j_{N, R_\beta}(N^{-\beta})}{f_\beta(N^{-\beta})} \leq 1$.

(g) Since f_β is a nonnegative, monotone nondecreasing function in $|x|$ with $f_\beta(x) = 1 \forall |x| \geq R_\beta$, it follows that

$$\begin{aligned} Cf_\beta(N^{-\beta}) &= f_\beta(N^{-\beta}) \int_{\mathbb{R}^2} d^2x V_N(x) \geq \int V_N(x) f_\beta(x) d^2x \\ &= \int_{\mathbb{R}^2} d^2x W_\beta(x) f_\beta(x) \geq f_\beta(N^{-\beta}) \int_{\mathbb{R}^2} d^2x W_\beta(x). \end{aligned}$$

Therefore, $\int_{\mathbb{R}^2} d^2x W_\beta(x) \leq CN$ holds, which implies that $R_\beta \leq CN^{1/2-\beta}$.

From

$$\begin{aligned} \frac{1}{K_\beta} \frac{4\pi}{N + \ln\left(\frac{R_\beta}{a}\right)} &= \frac{1}{K_\beta} \int_{\mathbb{R}^2} d^2x V_N(x) j_{N, R_\beta}(x) = \int_{\mathbb{R}^2} d^2x V_N(x) f_\beta(x) \\ &= \int_{\mathbb{R}^2} d^2x M_\beta(x) f_\beta(x) = 8\pi^2 N^{-1+2\beta} \int_{N^{-\beta}}^{R_\beta} dr r f_\beta(r) \end{aligned}$$

we conclude that

$$\int_{N^{-\beta}}^{R_\beta} dr r f_\beta(r) = \frac{N^{1-2\beta}}{2\pi K_\beta \left(N + \ln\left(\frac{R_\beta}{a}\right) \right)}.$$

Since f_β is a nonnegative, monotone nondecreasing function in $|x|$, for $N^{-\beta} \leq |x| \leq R_\beta$,

$$\frac{1}{2}(R_\beta^2 - N^{-2\beta}) \frac{j_{N, R_\beta}(N^{-\beta})}{K_\beta} = \frac{1}{2}(R_\beta^2 - N^{-2\beta}) f_\beta(N^{-\beta}) \leq \int_{N^{-\beta}}^{R_\beta} dr r f_\beta(r),$$

which implies

$$R_\beta^2 N^{2\beta} \leq \frac{N}{\pi \left(N + \ln\left(\frac{R_\beta}{a}\right) \right) j_{N, R_\beta}(N^{-\beta})} + 1.$$

Using $R_\beta \leq CN^{1/2-\beta}$, it then follows

$$j_{N, R_\beta}(N^{-\beta}) = 1 + \frac{1}{N + \ln\left(\frac{R_\beta}{a}\right)} \ln\left(\frac{N^{-\beta}}{R_\beta}\right) \geq 1 - \frac{C}{N},$$

which implies $R_\beta \leq CN^{-\beta}$.

(h) Using

$$\|M_\beta f_\beta\|_1 = \int_{\mathbb{R}^2} d^2x V_N(x) f_\beta(x) = K_\beta^{-1} \int_{\mathbb{R}^2} d^2x V_N(x) j_{N,R_\beta}(x) = K_\beta^{-1} \frac{4\pi}{N + \ln\left(\frac{R_\beta}{a}\right)},$$

we obtain (note that $a > 0$ holds)

$$\begin{aligned} \left| N \int_{\mathbb{R}^2} d^2x V_N(x) f_\beta(x) - 4\pi \right| &= |N\|M_\beta f_\beta\|_1 - 4\pi| = 4\pi \left| K_\beta^{-1} \frac{N}{N + \ln\left(\frac{R_\beta}{a}\right)} - 1 \right| \\ &= \frac{4\pi}{K_\beta} \left| \frac{N - NK_\beta + K_\beta \ln\left(\frac{R_\beta}{a}\right)}{N + \ln\left(\frac{R_\beta}{a}\right)} \right| \leq C \frac{\ln(N)}{N}. \end{aligned}$$

(i) Since $g_\beta(x) = 0$ for $|x| > R_\beta$, we conclude with $R_\beta \leq CN^{-\beta}$ that

$$\|g_\beta\|_1 \leq CN^{-2\beta},$$

as well as

$$\|g_\beta\| \leq CN^{-\beta}.$$

$\|g_\beta\|_\infty \leq 2$ follows from $g_\beta = 1 - f_\beta$ and the fact that f_β is a monotone nondecreasing function with $\|f_\beta\|_\infty = 1$.

(j) Using (h) and (i), we obtain with $\|M_\beta\|_1 \leq CN^{-1}$

$$\begin{aligned} |N\|M_\beta\|_1 - 4\pi| &\leq |N\|M_\beta f_\beta\|_1 - 4\pi| + N\|M_\beta g_\beta\|_1 \\ &\leq C \left(\frac{\ln(N)}{N} + \|\mathbf{1}_{|\cdot| \geq N^{-\beta}} g_\beta\|_\infty \right). \end{aligned}$$

For $N^{-\beta} \leq |x|$, $g_\beta(x)$ is a nonnegative, monotone nonincreasing function. It then follows with $K_\beta \leq 1$

$$\begin{aligned} \|\mathbf{1}_{|\cdot| \geq N^{-\beta}} g_\beta\|_\infty &= g_\beta(N^{-\beta}) = 1 - f_\beta(N^{-\beta}) = 1 - \frac{j_{N,R_\beta}(N^{-\beta})}{K_\beta} \\ &\leq 1 - \left(1 + \frac{1}{N + \ln\left(\frac{R_\beta}{a}\right)} \ln\left(\frac{N^{-\beta}}{R_\beta}\right) \right). \end{aligned}$$

and (j) follows.

(k) $M_\beta \in \mathcal{V}_\beta$ follows directly from $R_\beta \leq CN^{-\beta}$. Furthermore, $0 \leq M_\beta(x) f_\beta(x) \leq M_\beta(x)$ implies $M_\beta f_\beta \in \mathcal{V}_\beta$.

□

3.4 Proof of the Theorem

3.4.1 Proof for the potential W_β

Choosing the weight

We define a functional $\alpha : L^2(\mathbb{R}^{2N}, \mathbb{C}) \times L^2(\mathbb{R}^2, \mathbb{C}) \rightarrow \mathbb{R}_0^+$ such that

- (a) $\alpha(\Psi_t, \varphi_t)$ can be estimated via a Grönwall type estimate.
- (b) $\lim_{N \rightarrow \infty} \alpha(\Psi, \varphi) = 0$ implies convergence of the reduced one particle density matrix $\gamma_\psi^{(1)}$ to $|\varphi\rangle\langle\varphi|$ in trace norm.

Remark 3.4.1 In both this subsection and in Subsection 3.4.2, we will use the same definition of α as in [60]. There, the validity of the three-dimensional Gross-Pitaevskii equation was shown.

For $\beta > 0$ and N large, the interaction is strongly singular and one needs smoothness properties of Ψ_t to be able to control the dynamics of the condensate. This can be achieved by assuming closeness of the respective energies $|\mathcal{E}_{W_\beta}(\Psi_0) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi_0)|$. For $\beta < 1/2$ and many different choices of the weight, the following bound can be verified

$$\begin{aligned} \alpha(\Psi_t, \varphi_t) &\leq \alpha(\Psi_0, \varphi_0) \\ &+ \int_0^t ds \left(\mathcal{K}(\varphi_s, A_s) \left(\alpha(\Psi_s, \varphi_s) + \mathcal{O}(1) + \langle\langle \Psi_s, \widehat{n}^{\varphi_s} \Psi_t \rangle\rangle + |\mathcal{E}_{W_\beta}(\Psi_s) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi_s)| \right) \right), \end{aligned}$$

where we like to recall the notation $b_{W_\beta} = N \int_{\mathbb{R}^2} W_\beta(x) d^2x$. This enables us to perform an integral type Grönwall estimate, if we choose

$$\alpha(\Psi_t, \varphi_t) = \langle\langle \Psi_t, \widehat{n}^{\varphi_t} \Psi_t \rangle\rangle + |\mathcal{E}_{W_\beta}(\Psi_t) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi_t)|.$$

For $\beta \geq 1/2$, however, the time derivative of $\alpha(\Psi_t, \varphi_t)$, as just defined, cannot be bounded as stated above³. The reason for this is that the time derivative of $\langle\langle \Psi_t, \widehat{n}^{\varphi_t} \Psi_t \rangle\rangle$ contains the contributions $\widehat{n} - \widehat{n}_1$ and $\widehat{n} - \widehat{n}_2$. In several terms, it is then necessary to apply the bound $\|\widehat{n} - \widehat{n}_i\|_{\text{op}} = \mathcal{O}(N^{-1/2})$, $i = 1, 2$, which can be easily verified. To obtain a Grönwall estimate for $\beta \geq 1/2$, we define a weight function, which will be denoted by $m(k)$, such that $\|\widehat{m} - \widehat{m}_i\|_{\text{op}}$ yields to improved estimates.

Definition 3.4.2 For $0 < \xi < \frac{1}{2}$ define $m : \mathbb{N}_0 \rightarrow \mathbb{R}_0^+$,

$$m(k) = \begin{cases} \sqrt{k/N}, & \text{for } k \geq N^{1-2\xi}, \\ 1/2(N^{-1+\xi}k + N^{-\xi}), & \text{else.} \end{cases}$$

and

$$\alpha^<(\Psi, \varphi) = \langle\langle \Psi, \widehat{m}^\varphi \Psi \rangle\rangle + |\mathcal{E}_{W_\beta}(\Psi) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi)|.$$

³ It can be verified that in the case of $\alpha(\Psi_t, \varphi_t) = \langle\langle \Psi_t, \widehat{n}^{\varphi_t} \Psi_t \rangle\rangle + |\mathcal{E}_{W_\beta}(\Psi_t) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi_t)|$ the Estimate (3.68) given in Lemma 3.5.7, part (b) is not decaying in N .

With this definition, we obtain $N\|\widehat{m} - \widehat{m}_1\|_{\text{op}} \leq CN^\xi$, see (3.54).

Lemma 3.4.3 *Let $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C})$ and let $\varphi \in L^2(\mathbb{R}^2, \mathbb{C})$. Let $\alpha^<(\Psi, \varphi)$ be defined as above. Then,*

$$\begin{aligned} \lim_{N \rightarrow \infty} \alpha^<(\Psi, \varphi) = 0 &\Leftrightarrow \lim_{N \rightarrow \infty} \gamma_\Psi^{(1)} = |\varphi\rangle\langle\varphi| \text{ in trace norm} \\ \text{and } \lim_{N \rightarrow \infty} (\mathcal{E}_{W_\beta}(\Psi) - \mathcal{E}_{bW_\beta}^{GP}(\varphi)) &= 0. \end{aligned}$$

Proof: We prove $\lim_{N \rightarrow \infty} \langle\langle \Psi, \widehat{m}\Psi \rangle\rangle = 0 \Leftrightarrow \lim_{N \rightarrow \infty} \gamma_\Psi^{(1)} = |\varphi\rangle\langle\varphi|$ in trace norm. Using the inequality $\|\widehat{n} - \widehat{m}\|_{\text{op}} = N^{-\xi}$, we then obtain $\langle\langle \Psi, \widehat{m}\Psi \rangle\rangle \leq \langle\langle \Psi, q_1\Psi \rangle\rangle + N^{-\xi}$. The Lemma then follows together with Lemma 2.0.11. \square

To obtain the desired Grönwall estimate, we will calculate $\frac{d}{dt} \langle\langle \Psi_t, \widehat{m}^{\varphi_t} \Psi_t \rangle\rangle$ and $\frac{d}{dt} (\mathcal{E}_{W_\beta}(\Psi_t) - \mathcal{E}_{bW_\beta}^{GP}(\varphi_t))$. For this, define

Definition 3.4.4 *Let $W_\beta \in \mathcal{V}_\beta$ as in Definition 3.3.4. Define*

$$Z_\beta^\varphi(x_j, x_k) = W_\beta(x_j - x_k) - \frac{N \int_{\mathbb{R}^2} W_\beta(x) d^2x}{N-1} |\varphi|^2(x_j) - \frac{N \int_{\mathbb{R}^2} W_\beta(x) d^2x}{N-1} |\varphi|^2(x_k). \quad (3.26)$$

Note, for $W_\beta(x) = N^{-1+2\beta} W(N^\beta x)$, we have $N \int_{\mathbb{R}^2} W_\beta(x) d^2x = \int_{\mathbb{R}^2} W(x) d^2x$. With

$$m^a(k) = m(k) - m(k+1), \quad m^b(k) = m(k) - m(k+2)$$

and

$$\widehat{r} = \widehat{m}^b p_1 p_2 + \widehat{m}^a (p_1 q_2 + q_1 p_2),$$

we define the functionals $\gamma_{a,b}^< : L^2(\mathbb{R}^{2N}, \mathbb{C}) \times L^2(\mathbb{R}^2, \mathbb{C}) \rightarrow \mathbb{R}_0^+$ by

$$\gamma_a^<(\Psi, \varphi) = \langle\langle \Psi, \dot{A}_t(x_1) \Psi \rangle\rangle - \langle \varphi, \dot{A}_t \varphi \rangle \quad (3.27)$$

$$\gamma_b^<(\Psi, \varphi) = N(N-1) \Im (\langle\langle \Psi, Z_\beta^\varphi(x_1, x_2) \widehat{r} \Psi \rangle\rangle) \quad (3.28)$$

$$= -2N(N-1) \Im (\langle\langle \Psi, p_1 q_2 \widehat{m}_{-1}^a Z_\beta^\varphi(x_1, x_2) p_1 p_2 \Psi \rangle\rangle) \quad (3.29)$$

$$- N(N-1) \Im (\langle\langle \Psi, q_1 q_2 \widehat{m}_{-2}^b W_\beta(x_1 - x_2) p_1 p_2 \Psi \rangle\rangle) \quad (3.30)$$

$$- 2N(N-1) \Im (\langle\langle \Psi, q_1 q_2 \widehat{m}_{-1}^a Z_\beta^\varphi(x_1, x_2) p_1 q_2 \Psi \rangle\rangle). \quad (3.31)$$

Lemma 3.4.5 *Let $W_\beta \in \mathcal{V}_\beta$ as in Definition 3.3.4. Let Ψ_t the unique solution to $i\partial_t \Psi_t = H_{W_\beta} \Psi_t$ with initial datum $\Psi_0 \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap H^2(\mathbb{R}^{2N}, \mathbb{C})$, $\|\Psi_0\| = 1$. Let φ_t the unique solution to $i\partial_t \varphi_t = h_{bW_\beta}^{GP} \varphi_t$ with initial datum $\varphi_0 \in H^2(\mathbb{R}^2, \mathbb{C})$, $\|\varphi_0\| = 1$. Let $\alpha^<(\Psi_t, \varphi_t)$ be defined as in Definition 3.4.2. Then*

$$\alpha^<(\Psi_t, \varphi_t) \leq \alpha^<(\Psi_0, \varphi_0) + \int_0^t ds (|\gamma_a^<(\Psi_s, \varphi_s)| + |\gamma_b^<(\Psi_s, \varphi_s)|). \quad (3.32)$$

Proof: (see also Lemma 6.2. in [60]) The time derivative of φ_t is given by (3.3), i.e. $i\partial_t\varphi_t(x_j) = h_{b_{W_\beta},j}^{GP}\varphi_t(x_j)$. Here, $h_{b_{W_\beta},j}^{GP}$ denotes the operator $h_{b_{W_\beta}}^{GP}$ acting on the j^{th} coordinate x_j . We then obtain

$$\begin{aligned} & \frac{d}{dt} \langle\langle \Psi_t, \widehat{m}^{\varphi_t} \Psi_t \rangle\rangle \\ &= i \langle\langle H_{W_\beta} \Psi_t, \widehat{m}^{\varphi_t} \Psi_t \rangle\rangle - i \langle\langle \Psi_t, \widehat{m}^{\varphi_t} H_{W_\beta} \Psi_t \rangle\rangle - i \langle\langle \Psi_t, \left[\sum_{j=1}^N h_{b_{W_\beta},j}^{GP}, \widehat{m}^{\varphi_t} \right] \Psi_t \rangle\rangle \\ &= i \langle\langle \Psi_t, [H_{W_\beta} - \sum_{j=1}^N h_{b_{W_\beta},j}^{GP}, \widehat{m}^{\varphi_t}] \Psi_t \rangle\rangle = i \frac{N(N-1)}{2} \langle\langle \Psi_t, [Z_\beta^{\varphi_t}(x_1, x_2), \widehat{m}^{\varphi_t}] \Psi_t \rangle\rangle, \end{aligned}$$

where we used symmetry of Ψ_t in the last step. Using Lemma 2.0.5 (d), it follows that the latter equals (dropping the explicit dependence on φ_t from now on)

$$\begin{aligned} & \frac{d}{dt} \langle\langle \Psi_t, \widehat{m}^{\varphi_t} \Psi_t \rangle\rangle = i \frac{N(N-1)}{2} \langle\langle \Psi_t, [Z_\beta^{\varphi_t}(x_1, x_2), p_1 p_2 (\widehat{m} - \widehat{m}_2)] \Psi_t \rangle\rangle \\ &+ i \frac{N(N-1)}{2} \langle\langle \Psi_t, [Z_\beta^{\varphi_t}(x_1, x_2), (p_1 q_2 + q_1 p_2)(\widehat{m} - \widehat{m}_1)] \Psi_t \rangle\rangle. \end{aligned}$$

By a straightforward calculation, we obtain

$$\begin{aligned} & \frac{d}{dt} \langle\langle \Psi_t, \widehat{m}^{\varphi_t} \Psi_t \rangle\rangle = -N(N-1) \\ & \Im \left(\langle\langle \Psi_t, (p_1 p_2 + p_1 q_2 + q_1 p_2 + q_1 q_2) Z_\beta^{\varphi_t}(x_1, x_2) (\widehat{m}^b p_1 p_2 + \widehat{m}^a (p_1 q_2 + q_1 p_2)) \Psi_t \rangle\rangle \right). \end{aligned}$$

Note that in view of Lemma 2.0.5 (c) $\widehat{r} Q_j Z_\beta^{\varphi_t}(x_1, x_2) Q_j = Q_j Z_\beta^{\varphi_t}(x_1, x_2) Q_j \widehat{r}$ for any $j \in \{0, 1, 2\}$ and any weight r . Therefore,

$$\begin{aligned} & \Im \left(\langle\langle \Psi_t, p_1 p_2 Z_\beta^{\varphi_t}(x_1, x_2) \widehat{m}^b p_1 p_2 \Psi_t \rangle\rangle \right) = 0 \\ & \Im \left(\langle\langle \Psi_t, (p_1 q_2 + q_1 p_2) Z_\beta^{\varphi_t}(x_1, x_2) \widehat{m}^a (p_1 q_2 + q_1 p_2) \Psi_t \rangle\rangle \right) = 0. \end{aligned}$$

Using Symmetry and Lemma 2.0.5 (c), we obtain the first line (3.28). Furthermore,

$$\begin{aligned} & \frac{d}{dt} \langle\langle \Psi_t, \widehat{m}^{\varphi_t} \Psi_t \rangle\rangle = -2N(N-1) \Im \left(\langle\langle \Psi_t, \widehat{m}_{-1}^b p_1 q_2 Z_\beta^{\varphi_t}(x_1, x_2) p_1 p_2 \Psi_t \rangle\rangle \right) \\ & \quad - N(N-1) \Im \left(\langle\langle \Psi_t, \widehat{m}_{-2}^b q_1 q_2 Z_\beta^{\varphi_t}(x_1, x_2) p_1 p_2 \Psi_t \rangle\rangle \right) \\ & \quad - 2N(N-1) \Im \left(\langle\langle \Psi_t, p_1 p_2 Z_\beta^{\varphi_t}(x_1, x_2) \widehat{m}^a p_1 q_2 \Psi_t \rangle\rangle \right) \\ & \quad - 2N(N-1) \Im \left(\langle\langle \Psi_t, \widehat{m}_{-1}^a q_1 q_2 Z_\beta^{\varphi_t}(x_1, x_2) p_1 q_2 \Psi_t \rangle\rangle \right). \end{aligned}$$

Since $p_1 p_2 |\varphi_t^2|(x_1) q_1 q_2 = p_1 p_2 q_2 |\varphi_t^2|(x_1) q_1 = 0 = p_1 p_2 |\varphi_t^2|(x_2) q_1 q_2$, we can replace $Z_\beta^{\varphi_t}(x_1, x_2)$ in the second line by $W_\beta(x_1 - x_2)$. The third line equals

$$2N(N-1) \Im \left(\langle\langle \Psi, \widehat{m}^a p_1 q_2 Z_\beta^{\varphi_t}(x_1, x_2) p_1 p_2 \Psi \rangle\rangle \right).$$

Since

$$m(k-1) - m(k+1) - (m(k) - m(k+1)) = m(k-1) - m(k)$$

it follows that $\widehat{m}_{-1}^b - \widehat{m}^a = \widehat{m}_{-1}^a$ and we get

$$\begin{aligned} \frac{d}{dt} \langle\langle \Psi_t, \widehat{m}^{\varphi_t} \Psi_t \rangle\rangle &= -2N(N-1) \Im \left(\langle\langle \Psi, p_1 q_2 \widehat{m}_{-1}^a Z_{\beta}^{\varphi_t}(x_1, x_2) p_1 p_2 \Psi \rangle\rangle \right) \\ &\quad - N(N-1) \Im \left(\langle\langle \Psi, q_1 q_2 \widehat{m}_{-2}^b W_{\beta}(x_1 - x_2) p_1 p_2 \Psi \rangle\rangle \right) \\ &\quad - 2N(N-1) \Im \left(\langle\langle \Psi, q_1 q_2 \widehat{m}_{-1}^a Z_{\beta}^{\varphi_t}(x_1, x_2) p_1 q_2 \Psi \rangle\rangle \right). \end{aligned}$$

Furthermore,

$$\begin{aligned} \frac{d}{dt} \left(\mathcal{E}_{W_{\beta}}(\Psi_t) - \mathcal{E}_{b_{W_{\beta}}}^{GP}(\varphi_t) \right) &= \langle\langle \Psi_t, \dot{A}_t(x_1) \Psi_t \rangle\rangle - \langle \varphi_t, \dot{A}_t \varphi_t \rangle, \\ i \left\langle \varphi_t, \left[h_{b_{W_{\beta}}}^{GP}, \left(h_{b_{W_{\beta}}}^{GP} - \frac{b_{W_{\beta}}}{2} |\varphi_t|^2 \right) \right] \varphi_t \right\rangle &+ \left\langle \varphi_t, \frac{b_{W_{\beta}}}{2} \left(\frac{d}{dt} |\varphi_t|^2 \right) \varphi_t \right\rangle \\ &= \langle\langle \Psi_t, \dot{A}_t(x_1) \Psi_t \rangle\rangle - \langle \varphi_t, \dot{A}_t \varphi_t \rangle + i \left\langle \varphi_t, \left[h_{b_{W_{\beta}}}^{GP}, \frac{b_{W_{\beta}}}{2} |\varphi_t|^2 \right] \varphi_t \right\rangle \\ &\quad - i \left\langle \varphi_t, \left[h_{b_{W_{\beta}}}^{GP}, \frac{b_{W_{\beta}}}{2} |\varphi_t|^2 \right] \varphi_t \right\rangle = \gamma_a^<(\Psi_t, \varphi_t). \end{aligned}$$

The Lemma then follows using that $|f(x)| \leq |f(0)| + \int_0^x dy |f'(y)|$ holds for any $f \in C^1(\mathbb{R}, \mathbb{C})$.

□

Establishing the Grönwall estimate

Lemma 3.4.6 *Let $W_{\beta} \in \mathcal{V}_{\beta}$ as in Definition 3.3.4 and assume the operator inequality $-(1-\epsilon)\Delta + \frac{1}{2}W \geq 0$ on $L^2(\mathbb{R}^2, \mathbb{C})$ for some $\epsilon > 0$. Let Ψ_t the unique solution to $i\partial_t \Psi_t = H_{W_{\beta}} \Psi_t$ with initial datum $\Psi_0 \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap H^2(\mathbb{R}^{2N}, \mathbb{C})$, $\|\Psi_0\| = 1$. Let φ_t the unique solution to $i\partial_t \varphi_t = h_{b_{W_{\beta}}}^{GP} \varphi_t$ with initial datum $\varphi_0 \in H^3(\mathbb{R}^2, \mathbb{C})$. Let $\mathcal{E}_{W_{\beta}}(\Psi_0) \leq C$. Let $\gamma_a^<(\Psi_t, \varphi_t)$ and $\gamma_b^<(\Psi_t, \varphi_t)$ be defined as in Definition (3.4.4). Then, there exists an $\eta > 0$ such that*

$$\gamma_a^<(\Psi_t, \varphi_t) \leq C \|\dot{A}_t\|_{\infty} (\langle\langle \Psi_t, \widehat{m}^{\varphi_t} \Psi_t \rangle\rangle + N^{-\frac{1}{2}}), \quad (3.33)$$

$$\gamma_b^<(\Psi_t, \varphi_t) \leq \mathcal{K}(\varphi_t, A_t) \left(\langle\langle \Psi_t, \widehat{m}^{\varphi_t} \Psi_t \rangle\rangle + N^{-\eta} + \left| \mathcal{E}_{W_{\beta}}(\Psi_t) - \mathcal{E}_{b_{W_{\beta}}}^{GP}(\varphi_t) \right| \right). \quad (3.34)$$

The proof of this Lemma can be found in Section 3.5.4. Once we have proven Lemma 3.4.6, we obtain with Lemma 3.4.5, Grönwall's Lemma and the estimate above that

$$\begin{aligned} \alpha^<(\Psi_t, \varphi_t) &\leq e^{\int_0^t ds \mathcal{K}(\varphi_s, A_s)} \left(\alpha^<(\Psi_0, \varphi_0) \right. \\ &\quad \left. + \int_0^t ds \mathcal{K}(\varphi_s, A_s) e^{-\int_0^s d\tau \mathcal{K}(\varphi_{\tau}, A_{\tau})} N^{-\eta} \right). \end{aligned}$$

Note that under the assumptions $\varphi_t \in H^3(\mathbb{R}^2, \mathbb{C})$ and $A_t \in C^1(\mathbb{R}, L^\infty(\mathbb{R}^2, \mathbb{R}))$ there exists a constant $C_t < \infty$, depending on t , φ_0 and A_t , such that $\int_0^t ds \mathcal{K}(\varphi_s, A_s) \leq C_t$, see Lemma 3.6.1. This proves, using Lemma 3.4.3, part (a) of Theorem 3.2.5. If the potential is switched off, one expects that C_t is of order t since in this case $\|\varphi_t\|_\infty$ and $\|\nabla \varphi_t\|_\infty$ are expected to decay like t^{-1} .

We want to explain on a heuristic level why $\gamma_b^<(\Psi_t, \varphi_t)$ is small. The principle argument follows the ideas and estimates of [60]. The first line in (3.29) is only small if the correct coupling parameter b_{W_β} is used in the mean-field equation (3.3). Then,

$$N p_1 W_\beta(x_1 - x_2) p_1 = N p_1 W_\beta \star |\varphi|^2(x_2) p_1 \rightarrow b_{W_\beta} p_1 |\varphi|^2(x_2)$$

converges against the mean-field potential, and hence the first expression of (3.29) can be estimated sufficiently well. In order to bound the second and third line of (3.29), one tries to bound $N^2 \langle\langle \Psi, q_1 q_2 \hat{m}_{-2}^b W_\beta(x_1 - x_2) p_1 p_2 \Psi \rangle\rangle$ and $N^2 \langle\langle \Psi, q_1 q_2 \hat{m}_{-1}^a W_\beta(x_1 - x_2) p_1 q_2 \Psi \rangle\rangle$ in terms of $\langle\langle \Psi, \hat{n} \Psi \rangle\rangle + \mathcal{O}(N^{-\eta})$ for some $\eta > 0$. For large β , one needs to use additional smoothness properties of Ψ . This explains the appearance on $|\mathcal{E}_{W_\beta}(\Psi_0) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi_0)|$ on the right hand side of (3.34). The concise estimates are quite involved and can be found in Section 3.5.4.

3.4.2 Proof for the exponential scaling V_N

Adapting the weight

To control the dynamics generated by H_{V_N} , it is necessary to modify the counting functional $\alpha^<(\Psi, \varphi)$ in order to obtain the desired Grönwall estimate. $\gamma_b^<(\Psi, \varphi)$, which was defined in (3.29), will not be small if we were to replace W_β by V_N . In particular, $\|V_N\| = \mathcal{O}(e^N)$, which would appear in the respective estimates, cannot be bounded by any finite polynomial in $1/N$. In order to control the dynamics of the condensate, one needs to account for the microscopic structure which is induced by V_N , as explained in Section 3.3. The idea we will employ is the following: For the moment, we will consider the most simple counting functional $\langle\langle \Psi_t, q_1^{\varphi_t} \Psi_t \rangle\rangle = 1 - \langle\langle \Psi_t, p_1^{\varphi_t} \Psi_t \rangle\rangle$. This functional counts the relative number of particles which are not in the state φ_t . Instead of projecting onto φ_t , we now consider the functional

$$1 - \langle\langle \Psi_t, \prod_{j=2}^N f_\beta(x_1 - x_j) p_1^{\varphi_t} \prod_{j=2}^N f_\beta(x_1 - x_j) \Psi_t \rangle\rangle,$$

which takes the short scale correlation structure into account. Neglecting all but two-particle interactions, this can be approximated by

$$\begin{aligned} 1 - \langle\langle \Psi_t, \left(1 - \sum_{j=2}^N g_\beta(x_1 - x_j)\right) p_1^{\varphi_t} \left(1 - \sum_{l=2}^N g_\beta(x_1 - x_l)\right) \Psi_t \rangle\rangle \\ \approx \langle\langle \Psi_t, q_1^{\varphi_t} \Psi_t \rangle\rangle + 2(N-1) \Re(\langle\langle \Psi_t, g_\beta(x_1 - x_2) p_1^{\varphi_t} \Psi_t \rangle\rangle). \end{aligned}$$

The time derivative of this functional yields to the replacement of V_N by M_β and one obtains a similar contribution as in Definition 3.4.4. In addition, one obtains several other terms, which need to be estimated. The strategy we are going to employ is thus to estimate the time derivative of the modified functional and to show that we obtain a Grönwall estimate. Note, that, using Lemma 2.0.5 (e) with Lemma 3.3.6 (i)

$$2(N-1) |\Re(\langle\langle \Psi_t, g_\beta(x_1 - x_2) p_1^{\varphi_t} \Psi_t \rangle\rangle)| \leq CN \|\varphi_t\|_\infty \|g_\beta\| \leq C \|\varphi_t\|_\infty N^{1-\beta}$$

holds. Hence, we obtain the a priori estimate

$$\langle\langle \Psi_t, q_1^{\varphi_t} \Psi_t \rangle\rangle \leq \langle\langle \Psi_t, q_1^{\varphi_t} \Psi_t \rangle\rangle + 2(N-1) \Re(\langle\langle \Psi_t, g_\beta(x_1 - x_2) p_1^{\varphi_t} \Psi_t \rangle\rangle) + C \|\varphi_t\|_\infty N^{1-\beta},$$

which explains why, for $\beta > 1$, the new defined functional implies convergence of the reduced density matrix $\gamma_{\Psi_t}^{(1)}$ to $|\varphi_t\rangle\langle\varphi_t|$ in trace norm.

We now adapt the strategy explained above to modify the counting functional $\alpha^<(\Psi, \varphi)$.

Definition 3.4.7 Let $\hat{r} = \hat{m}^b p_1 p_2 + \hat{m}^a (p_1 q_2 + q_1 p_2)$. Let $\beta > 6$ and let the functional $\alpha : L^2(\mathbb{R}^{2N}, \mathbb{C}) \times L^2(\mathbb{R}^2, \mathbb{C}) \rightarrow \mathbb{R}_0^+$ be defined by

$$\alpha(\Psi, \varphi) = \langle\langle \Psi, \hat{m} \Psi \rangle\rangle + \left| \mathcal{E}_{V_N}(\Psi) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi) \right| - N(N-1) \Re(\langle\langle \Psi, g_\beta(x_1 - x_2) \hat{r} \Psi \rangle\rangle) \quad (3.35)$$

and the functional $\gamma : L^2(\mathbb{R}^{2N}, \mathbb{C}) \times L^2(\mathbb{R}^2, \mathbb{C}) \rightarrow \mathbb{R}$ be defined by

$$\gamma(\Psi, \varphi) = |\gamma_a(\Psi, \varphi)| + |\gamma_b(\Psi, \varphi)| + |\gamma_c(\Psi, \varphi)| + |\gamma_d(\Psi, \varphi)| + |\gamma_e(\Psi, \varphi)| + |\gamma_f(\Psi, \varphi)|, \quad (3.36)$$

where the different summands are:

(a) The change in the energy-difference

$$\gamma_a(\Psi, \varphi) = \langle\langle \Psi, \dot{A}_t(x_1) \Psi \rangle\rangle - \langle \varphi, \dot{A}_t \varphi \rangle.$$

(b) The new interaction term

$$\begin{aligned} \gamma_b(\Psi, \varphi) = & -N(N-1) \Im \left(\langle\langle \Psi, \tilde{Z}_\beta^\varphi(x_1, x_2) \hat{r} \Psi \rangle\rangle \right) \\ & - N(N-1) \Im \left(\langle\langle \Psi, g_\beta(x_1 - x_2) \hat{r} \mathcal{Z}^\varphi(x_1, x_2) \Psi \rangle\rangle \right), \end{aligned}$$

where, using M_β from Definition 3.3.5,

$$\tilde{Z}_\beta^\varphi(x_1, x_2) = \left(M_\beta(x_1 - x_2) - b_{V_N} \frac{|\varphi|^2(x_1) + |\varphi|^2(x_2)}{N-1} \right) f_\beta(x_1 - x_2) \quad (3.37)$$

$$\mathcal{Z}^\varphi(x_1, x_2) = V_N(x_1 - x_2) - \frac{b_{V_N}}{N-1} |\varphi|^2(x_1) - \frac{b_{V_N}}{N-1} |\varphi|^2(x_2).$$

(c) The mixed derivative term

$$\gamma_c(\Psi, \varphi) = -4N(N-1) \langle\langle \Psi, (\nabla_1 g_\beta(x_1 - x_2)) \nabla_1 \hat{r} \Psi \rangle\rangle.$$

(d) *Three particle interactions*

$$\begin{aligned}\gamma_d(\Psi, \varphi) = & 2N(N-1)(N-2)\Im(\langle\langle \Psi, g_\beta(x_1 - x_2) [V_N(x_1 - x_3), \hat{r}] \Psi \rangle\rangle) \\ & + N(N-1)(N-2)\Im(\langle\langle \Psi, g_\beta(x_1 - x_2) [b_{V_N}|\varphi|^2(x_3), \hat{r}] \Psi \rangle\rangle).\end{aligned}$$

(e) *Interaction terms of the correction*

$$\gamma_e(\Psi, \varphi) = \frac{1}{2}N(N-1)(N-2)(N-3)\Im(\langle\langle \Psi, g_\beta(x_1 - x_2) [V_N(x_3 - x_4), \hat{r}] \Psi \rangle\rangle).$$

(f) *Correction terms of the mean field*

$$\gamma_f(\Psi, \varphi) = 2N(N-1)\frac{N-2}{N-1}\Im(\langle\langle \Psi, g_\beta(x_1 - x_2) [b_{V_N}|\varphi|^2(x_1), \hat{r}] \Psi \rangle\rangle).$$

Remark 3.4.8 (a) Recall that b_{V_N} is 4π in the case $a > 0$ and 0 in the case $a = 0$. In the latter case $M_\beta = 0$, $f_\beta = j_{N,\mathcal{R}}$ holds.

(b) The condition $\beta > 6$ implies the bound

$$|\gamma_c(\Psi, \varphi)| + |\gamma_d(\Psi, \varphi)| + |\gamma_e(\Psi, \varphi)| + |\gamma_f(\Psi, \varphi)| \leq \mathcal{K}(\varphi, A.)N^{-\delta}, \quad \delta > 0,$$

see (3.103).

(c) The functionals $\alpha(\Psi, \varphi)$ and $\gamma(\Psi, \varphi)$ defined above also appear in the derivation of the three dimensional Gross-Pitaevskii equation, see [60].

Lemma 3.4.9 Let Ψ_t the unique solution to $i\partial_t \Psi_t = H_{V_N} \Psi_t$ with initial datum $\Psi_0 \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap H^2(\mathbb{R}^{2N}, \mathbb{C})$, $\|\Psi_0\| = 1$. Let φ_t the unique solution to $i\partial_t \varphi_t = h_{b_{V_N}}^{GP} \varphi_t$ with initial datum $\varphi_0 \in H^2(\mathbb{R}^2, \mathbb{C})$, $\|\varphi_0\| = 1$. Let $\alpha(\Psi_t, \varphi_t)$ and $\gamma(\Psi_t, \varphi_t)$ be defined as in (3.35) and (3.36). Then

$$\alpha(\Psi_t, \varphi_t) \leq \alpha(\Psi_0, \varphi_0) + \int_0^t ds \gamma(\Psi_s, \varphi_s).$$

Proof: (see also Lemma 6.3. in [60]) We first calculate

$$\begin{aligned}\frac{d}{dt} (\langle\langle \Psi, \hat{m} \Psi \rangle\rangle - N(N-1)\Re(\langle\langle \Psi, g_\beta(x_1 - x_2) \hat{r} \Psi \rangle\rangle)) \\ = -N(N-1)\Im(\langle\langle \Psi_t, \mathcal{Z}^{\varphi_t}(x_1, x_2) \hat{r} \Psi_t \rangle\rangle) \\ - N(N-1)\Re\left(i\langle\langle \Psi_t, g_\beta(x_1 - x_2) \left[H_{V_N} - \sum_{i=1}^N h_{b_{V_N},i}^{GP}, \hat{r}\right] \Psi_t \rangle\rangle\right) \\ - N(N-1)\Re(i\langle\langle \Psi_t, [H_{V_N}, g_\beta(x_1 - x_2)] \hat{r} \Psi_t \rangle\rangle).\end{aligned}$$

Using symmetry, we obtain

$$\begin{aligned}
& \frac{d}{dt} (\langle\langle \Psi, \hat{m} \Psi \rangle\rangle - N(N-1)\Re(\langle\langle \Psi, g_\beta(x_1 - x_2) \hat{r} \Psi \rangle\rangle)) \\
&= -N(N-1)\Im(\langle\langle \Psi_t, \mathcal{Z}^{\varphi_t}(x_1, x_2) \hat{r} \Psi_t \rangle\rangle) \\
&\quad + N(N-1)\Im(\langle\langle \Psi_t, g_\beta(x_1 - x_2) [\mathcal{Z}^{\varphi_t}(x_1, x_2), \hat{r}] \Psi_t \rangle\rangle) \\
&\quad + 2N(N-1)(N-2)\Im(\langle\langle \Psi_t, g_\beta(x_1 - x_2) [V_N(x_1 - x_3), \hat{r}] \Psi_t \rangle\rangle) \\
&\quad + N(N-1)(N-2)\Im(\langle\langle \Psi_t, g_\beta(x_1 - x_2) [b_{V_N}|\varphi_t|^2(x_3), \hat{r}] \Psi_t \rangle\rangle) \\
&\quad + \frac{1}{2}N(N-1)(N-2)(N-3)\Im(\langle\langle \Psi_t, g_\beta(x_1 - x_2) [V_N(x_3 - x_4), \hat{r}] \Psi_t \rangle\rangle) \\
&\quad + N(N-1)\Im(\langle\langle \Psi_t, [H_{V_N}, g_\beta(x_1 - x_2)] \hat{r} \Psi_t \rangle\rangle) \\
&\quad + 2N(N-1)\frac{N-2}{N-1}\Im(\langle\langle \Psi_t, g_\beta(x_1 - x_2) [b_{V_N}|\varphi_t|^2(x_1), \hat{r}] \Psi_t \rangle\rangle).
\end{aligned}$$

The second and third lines equal γ_d (recall that Ψ is symmetric), the fourth line equals γ_e and the sixth line equals γ_f . Using that $(1 - g_\beta(x_1 - x_2))\mathcal{Z}^\varphi(x_1, x_2) = \tilde{Z}_\beta^\varphi(x_1, x_2) + (V_N(x_1 - x_2) - M_\beta(x_1 - x_2))f_\beta(x_1 - x_2)$ we get

$$\begin{aligned}
& \frac{d}{dt} (\langle\langle \Psi, \hat{m} \Psi \rangle\rangle - N(N-1)\Re(\langle\langle \Psi, g_\beta(x_1 - x_2) \hat{r} \Psi \rangle\rangle)) \\
&\leq \gamma_d(\Psi_t, \varphi_t) + \gamma_e(\Psi_t, \varphi_t) + \gamma_f(\Psi_t, \varphi_t) \\
&\quad - N(N-1)\Im(\langle\langle \Psi_t, \tilde{Z}_\beta^{\varphi_t}(x_1, x_2) \hat{r} \Psi_t \rangle\rangle) \\
&\quad - N(N-1)\Im(\langle\langle \Psi_t, (V_N(x_1 - x_2) - M_{\beta_1}(x_1 - x_2))f_\beta(x_1 - x_2) \hat{r} \Psi_t \rangle\rangle) \\
&\quad - N(N-1)\Im(\langle\langle \Psi_t, g_\beta(x_1 - x_2) \hat{r} \mathcal{Z}^{\varphi_t}(x_1, x_2) \Psi_t \rangle\rangle) \\
&\quad + N(N-1)\Im(\langle\langle \Psi_t, [H_{V_N}, g_\beta(x_1 - x_2)] \hat{r} \Psi_t \rangle\rangle).
\end{aligned} \tag{3.38}$$

The first, second and the fourth line yield to the contribution $\gamma_b + \gamma_d + \gamma_e + \gamma_f$. Using (3.3.5) the commutator in the fifth line equals

$$\begin{aligned}
[H_{V_N}, g_\beta(x_1 - x_2)] &= -[H_{V_N}, f_\beta(x_1 - x_2)] \\
&= [\Delta_1 + \Delta_2, f_\beta(x_1 - x_2)] \\
&= (\Delta_1 + \Delta_2)f_\beta(x_1 - x_2) \\
&\quad + (2\nabla_1 f_\beta(x_1 - x_2))\nabla_1 + (2\nabla_2 f_\beta(x_1 - x_2))\nabla_2 \\
&= (V_N(x_1 - x_2) - M_\beta(x_1 - x_2))f_\beta(x_1 - x_2) \\
&\quad - (2\nabla_1 g_\beta(x_1 - x_2))\nabla_1 - (2\nabla_2 g_\beta(x_1 - x_2))\nabla_2.
\end{aligned}$$

The third and fifth line in (3.38) then yield to

$$-4N(N-1)\langle\langle \Psi_t, (\nabla_1 g_\beta(x_1 - x_2))\nabla_1 \hat{r} \Psi_t \rangle\rangle = \gamma_c(\Psi_t, \varphi_t).$$

Using

$$\frac{d}{dt} (\mathcal{E}_{V_N}(\Psi_t) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi_t)) = \gamma_a(\Psi_t, \varphi_t),$$

we obtain the desired result.

□

Establishing the Grönwall estimate

Again, we will bound the time derivative of $\alpha(\Psi_t, \varphi_t)$ such that we can employ a Grönwall estimate.

Lemma 3.4.10 *Let Ψ_t the unique solution to $i\partial_t \Psi_t = H_{V_N} \Psi_t$ with initial datum $\Psi_0 \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap H^2(\mathbb{R}^{2N}, \mathbb{C})$, $\|\Psi_0\| = 1$. Let φ_t the unique solution to $i\partial_t \varphi_t = h_{b_{V_N}}^{GP} \varphi_t$ with initial datum $\varphi_0 \in H^3(\mathbb{R}^2, \mathbb{C})$. Let $\mathcal{E}_{V_N}(\Psi_0) \leq C$. Let $\gamma(\Psi_t, \varphi_t)$ be defined as in (3.36).*

(a) *There exists an $\eta > 0$ such that*

$$\gamma(\Psi_t, \varphi_t) \leq \mathcal{K}(\varphi_t, A_t) \left(\langle\langle \Psi_t, \widehat{n} \Psi_t \rangle\rangle + N^{-\eta} + \left| \mathcal{E}_{V_N}(\Psi_0) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi_0) \right| \right). \quad (3.39)$$

(b) *Let $\gamma(\Psi_t, \varphi_t)$ fulfill the Bound (3.39) given above. Let $\varphi_t \in H^3(\mathbb{R}^2, \mathbb{C})$ and let $A_t \in C^1(\mathbb{R}, L^\infty(\mathbb{R}^2, \mathbb{R}))$. Then,*

$$\lim_{N \rightarrow \infty} \left\| \gamma_{\Psi_t}^{(1)} - |\varphi_t\rangle\langle\varphi_t| \right\|_{tr} = 0 \quad (3.40)$$

holds.

Proof:

- (a) The proof of part (a) can be found in Section 3.5.5. We will shortly comment on the strategy to prove the bound given by Eq. (3.39). The most important estimate is γ_b , which can be estimated in the same way as $\gamma_b^<$. All other estimates are based on the smallness of the L^p -norms of g_β , see Lemma 3.3.6.
- (b) We show that Lemma 3.4.10, part (a) implies convergence of the reduced density matrix $\gamma_{\Psi_t}^{(1)}$ to $|\varphi_t\rangle\langle\varphi_t|$ in trace norm. Using $\|\widehat{m}^a\|_{\text{op}} + \|\widehat{m}^b\|_{\text{op}} \leq CN^{-1+\xi}$, see (3.54), together with Equation (2.4) and Lemma 3.3.6 (i), we obtain

$$\begin{aligned} \|g_\beta(x_1 - x_2)\widehat{r}\|_{\text{op}} &\leq \|g_\beta(x_1 - x_2)p_1(\widehat{m}^b p_2 + \widehat{m}^a q_2)\|_{\text{op}} + \|g_\beta(x_1 - x_2)p_2 q_1 \widehat{m}^a\|_{\text{op}} \\ &\leq \mathcal{K}(\varphi, A.) \|g_\beta\| (\|\widehat{m}^a\|_{\text{op}} + \|\widehat{m}^b\|_{\text{op}}) \leq \mathcal{K}(\varphi, A.) N^{\xi-1-\beta}. \end{aligned}$$

Therefore, we bound

$$N(N-1) |\Re(\langle\Psi, g_\beta(x_1 - x_2)\widehat{r}\Psi\rangle)| \leq \mathcal{K}(\varphi, A.) N^{1-\beta+\xi}. \quad (3.41)$$

For β large enough, (3.39) implies together with (3.41) that

$$\gamma(\Psi_t, \varphi_t) \leq \mathcal{K}(\varphi_t, A_t) (\alpha(\Psi_t, \varphi_t) + N^{-\eta}),$$

for some $\eta > 0$. We get with Lemma 3.4.5 and Grönwall's Lemma, using (3.41) again, that part (a) implies

$$\begin{aligned}\alpha^<(\Psi_t, \varphi_t) &\leq e^{\int_0^t ds \mathcal{K}(\varphi_s, A_s)} \left(\alpha^<(\Psi_0, \varphi_0) \right. \\ &\quad \left. + \int_0^t ds \mathcal{K}(\varphi_s, A_s) e^{-\int_0^s d\tau \mathcal{K}(\varphi_\tau, A_\tau)} N^{-\eta} \right).\end{aligned}$$

By Lemma 3.4.3, we then obtain convergence in trace norm of the respective density matrices.

□

With Lemma 3.4.10, we then obtain part (b) of Theorem 3.2.5. In the remaining part of this chapter, we will present the necessary proofs to conclude the main Theorem 3.2.5.

3.5 Rigorous estimates

3.5.1 Control on the kinetic energy of Ψ_t

We will prove that $\|\nabla_1 \Psi_t\|$ is uniformly bounded in N , if initially the energy per particle $\mathcal{E}_U(\Psi_0)$ is of order one. Under the assumption $\lim_{N \rightarrow \infty} (\mathcal{E}_{W_\beta}(\Psi_0) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi_0)) = 0$ (see Theorem 3.2.5), it immediately follows that $\mathcal{E}_{W_\beta}(\Psi_0) \leq C$. Similarly, the condition $\lim_{N \rightarrow \infty} (\mathcal{E}_{V_N}(\Psi_0) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi_0)) = 0$ implies $\mathcal{E}_{V_N}(\Psi_0) \leq C$. Furthermore, the operator inequality $-(1 - \epsilon)\Delta + \frac{1}{2}W \geq 0$, as well the Assumption 3.2.3 on V will be applied to show stability of second kind of the Hamiltonian $H_U, U \in \{W_\beta, V_N\}$. Note that it is sufficient to consider potentials W_β which scale like $W_\beta(x) = N^{-1+2\beta}W(N^\beta x)$ to prove Theorem 3.2.5, part (a).

Lemma 3.5.1 *Let $\Psi_0 \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap H^2(\mathbb{R}^{2N}, \mathbb{C})$ with $\|\Psi_0\| = 1$.*

(a) *Let $\beta > 0$, $W_\beta(x) = N^{-1+2\beta}W(N^\beta x)$ for $W \in L_c^\infty(\mathbb{R}^2, \mathbb{R})$, W spherically symmetric. Assume $-(1 - \epsilon)\Delta + \frac{1}{2}W \geq 0$ for some $\epsilon > 0$. Let Ψ_t the unique solution to $i\partial_t \Psi_t = H_{W_\beta} \Psi_t$ with initial datum Ψ_0 and let $\mathcal{E}_{W_\beta}(\Psi_0) \leq C$. Then*

$$\|\nabla_1 \Psi_t\| \leq \mathcal{K}(\varphi_t, A_t).$$

(b) *Let V satisfy Assumption 3.2.3. Let Ψ_t the unique solution to $i\partial_t \Psi_t = H_{V_N} \Psi_t$ with initial datum Ψ_0 and let $\mathcal{E}_{V_N}(\Psi_0) \leq C$. Then*

$$\|\nabla_1 \Psi_t\| \leq \mathcal{K}(\varphi_t, A_t).$$

Proof:

(a) Using $\frac{d}{dt}\mathcal{E}_{W_\beta}(\Psi_t) \leq \|\dot{A}_t\|_\infty$, we obtain $\mathcal{E}_{W_\beta}(\Psi_t) \leq \mathcal{K}(\varphi_t, A_t)$. By rescaling, the inequality $-(1-\epsilon)\Delta + \frac{1}{2}W \geq 0$, implies

$$-\epsilon\Delta_x \leq -\Delta_x + \frac{1}{2}(N-1)W_\beta(x-s),$$

with $s \in \mathbb{R}^2$ arbitrary.

We continue with

$$\begin{aligned} \epsilon \sum_{k=1}^N (-\Delta_k) &= \frac{1}{N-1} \sum_{i=1}^N \sum_{j=1, j \neq i}^N (-\epsilon\Delta_i) \\ &\leq \frac{1}{N-1} \sum_{i=1}^N \sum_{j=1, j \neq i}^N \left(-\Delta_i + \frac{1}{2}(N-1)W_\beta(x_i - x_j) \right) \\ &= \sum_{k=1}^N (-\Delta_k) + \sum_{i < j}^N W_\beta(x_i - x_j). \end{aligned} \tag{3.42}$$

We then obtain together with the assumption $A_t \in L^\infty(\mathbb{R}^2, \mathbb{R})$ that

$$\epsilon \langle\langle \Psi_t, -\Delta_1 \Psi_t \rangle\rangle \leq \frac{1}{N} \langle\langle \Psi_t, H_{W_\beta} \Psi_t \rangle\rangle + C \|A_t\|_\infty \leq \mathcal{K}(\varphi_t, A_t).$$

This yields the desired bound.

(b) is proven in Lemma 4.3.19.

□

3.5.2 Smoothing of the potential W_β

In Section 3.3 we have defined the potential M_β to control the strongly peaked potential V_N . We will employ a similar strategy to estimate the potential W_β sufficiently well when β is large. For this, we define, for $\beta_1 < \beta$, a potential $U_{\beta_1, \beta} \in \mathcal{V}_{\beta_1}$ such that $\int_{\mathbb{R}^2} W_\beta(x) d^2x = \|U_{\beta_1, \beta}\|_1$. Furthermore, define $h_{\beta_1, \beta}$ by $\Delta h_{\beta_1, \beta} = W_\beta - U_{\beta_1, \beta}$. The function $h_{\beta_1, \beta}$ can be thought as an electrostatic potential which is caused by the charge $W_\beta - U_{\beta_1, \beta}$. It is possible to rewrite

$$\begin{aligned} \langle\langle \chi, W_\beta(x_1 - x_2) \Omega \rangle\rangle &= \langle\langle \chi, U_{\beta_1, \beta}(x_1 - x_2) \Omega \rangle\rangle \\ &\quad - \langle\langle \nabla_1 \chi, (\nabla_1 h_{\beta_1, \beta})(x_1 - x_2) \Omega \rangle\rangle - \langle\langle \chi, (\nabla_1 h_{\beta_1, \beta})(x_1 - x_2) \nabla_1 \Omega \rangle\rangle, \end{aligned}$$

for $\chi, \omega \in L_s^2(\mathbb{R}^{2N}, \mathbb{C})$. We will verify that the L^p -norms of $h_{\beta_1, \beta}$ and $\nabla h_{\beta_1, \beta}$ are better to control than the respective L^p -norm of W_β . With additional control of $\nabla_1 \Omega$ and $\nabla_1 \chi$, it is therefore possible to obtain a sufficient bound for $\langle\langle \chi, W_\beta(x_1 - x_2) \Omega \rangle\rangle$ for large β .

Definition 3.5.2 For any $0 \leq \beta_1 \leq \beta$ and any $W_\beta \in \mathcal{V}_\beta$, as in Definition 3.3.4, we define

$$U_{\beta_1, \beta}(x) = \begin{cases} \frac{1}{\pi} \int_{\mathbb{R}^2} d^2x W_\beta(x) N^{2\beta_1} & \text{for } |x| < N^{-\beta_1}, \\ 0 & \text{else.} \end{cases}$$

and

$$h_{\beta_1, \beta}(x) = -\frac{1}{2\pi} \int_{\mathbb{R}^2} \ln|x-y| (W_\beta(y) - U_{\beta_1, \beta}(y)) d^2y. \quad (3.43)$$

Lemma 3.5.3 For any $0 \leq \beta_1 \leq \beta$ and any $W_\beta \in \mathcal{V}_\beta$, we obtain with the above definition

(a)

$$\begin{aligned} U_{\beta_1, \beta} &\in \mathcal{V}_{\beta_1}, \\ \Delta h_{\beta_1, \beta} &= W_\beta - U_{\beta_1, \beta}. \end{aligned}$$

(b) Pointwise estimates

$$|h_{\beta_1, \beta}(x)| \leq CN^{-1} \ln(N), \quad h_{\beta_1, \beta}(x) = 0 \text{ for } |x| \geq N^{-\beta_1}, \quad (3.44)$$

$$|\nabla h_{\beta_1, \beta}(x)| \leq CN^{-1} (|x|^2 + N^{-2\beta})^{-\frac{1}{2}}. \quad (3.45)$$

(c) Norm estimates

$$\begin{aligned} \|h_{\beta_1, \beta}\|_\infty &\leq CN^{-1} \ln(N), \\ \|h_{\beta_1, \beta}\|_\lambda &\leq CN^{-1-\frac{2}{\lambda}\beta_1} \ln(N) \text{ for } 1 \leq \lambda \leq \infty, \\ \|\nabla h_{\beta_1, \beta}\|_\lambda &\leq CN^{-1+\beta-\frac{2}{\lambda}\beta_1} \text{ for } 1 \leq \lambda \leq \infty. \end{aligned}$$

Furthermore, for $\lambda = 2$, we obtain the improved bounds

$$\|h_{0, \beta}\| \leq CN^{-1} \text{ for } \beta > 0, \quad (3.46)$$

$$\|\nabla h_{\beta_1, \beta}\| \leq CN^{-1} (\ln(N))^{1/2}. \quad (3.47)$$

Proof:

(a) $U_{\beta_1, \beta} \in \mathcal{V}_{\beta_1}$ follows directly from the definition of $U_{\beta_1, \beta}$.

The second statement is a well known result of standard electrostatics (therefore recall that the radially symmetric Greens function of the Laplace operator in two dimensions is given by $-\frac{1}{2\pi} \ln|x-y|$). W_β can be understood as a given charge density. $-U_{\beta_1, \beta}$ then corresponds to a smeared out charge density of opposite sign such that the “total charge” is zero. Hence, the “potential” $h_{\beta_1, \beta}$ can be chosen to be zero outside the support of the total charge density.⁴

⁴To see this, recall that the solution of $\Delta h(r) = \rho(r)$ for radially symmetric and regular enough charge density ρ is given by

$$h(r) = \ln(r) \int_0^r r' \rho(r') dr' + \int_r^\infty \ln(r') \rho(r') r' dr' + C,$$

where $C \in \mathbb{R}$. The r.h.s. is zero for $r \notin \text{supp}(\rho)$ when the total charge vanishes $\int_0^\infty r \rho(r) dr = 0$ and C is chosen equal to zero.

(b) We estimate the two terms on the r.h.s. of

$$h_{\beta_1, \beta}(x) = -\frac{1}{2\pi} \int_{\mathbb{R}^2} \ln|x-y| (W_\beta(y) - U_{\beta_1, \beta}(y)) d^2y$$

separately. $|h_{\beta_1, \beta}(x)| = 0$ as well as $W_\beta(x) - U_{\beta_1, \beta}(x) = 0$ for $|x| \geq N^{-\beta_1}$ implies that, whenever $|h_{\beta_1, \beta}(x)|$ is nonzero, $|x-y| \leq 1$ and therefore $-\ln|x-y| \geq 0$ in (3.43). Let $2RN^{-\beta} \leq |x|$. Since $-\ln|x-y| > 0$ in the support of U_β together with the support properties of W_β , one finds that for $RN^{-\beta} < |x|$

$$\frac{1}{2\pi} \int |\ln|x-y|| |W_\beta(y)| d^2y \leq C \|W_\beta\|_1 |\ln(|x| - RN^{-\beta})|,$$

which in turn implies

$$|h_{\beta_1, \beta}(x)| \leq C (\|W_\beta\|_1 + \|U_{\beta_1, \beta}\|_1) \ln N \leq CN^{-1} \ln(N)$$

for all $2RN^{-\beta} \leq |x|$.

Let next $|x| \leq 2RN^{-\beta}$. Here, one finds

$$\begin{aligned} \frac{1}{2\pi} \int |\ln|x-y|| |W_\beta(y)| d^2y &\leq C \|W_\beta\|_\infty \int_{B_{RN^{-\beta}(0)}} -\ln(|x-y|) d^2y \\ &\leq CN^{-1+2\beta} \int_{B_{RN^{-\beta}(x)}} -\ln|y| d^2y \leq CN^{-1+2\beta} \int_{B_{4RN^{-\beta}(0)}} -\ln|y| d^2y \\ &= CN^{-1+2\beta} \left[-|y|^2 (2 \ln|y| - 1) \right]_0^{4RN^{-\beta}} \leq CN^{-1} \ln(N^\beta), \end{aligned}$$

which implies for $|x| \leq 2RN^{-\beta}$

$$|h_{\beta_1, \beta}(x)| \leq N^{-1} \ln(N).$$

This proves the first statement.

For the gradient, we again estimate the two terms on the r.h.s. of

$$|\nabla h_{\beta_1, \beta}(x)| \leq \frac{1}{2\pi} \int \frac{1}{|x-y|} |W_\beta(y)| d^2y + \frac{1}{2\pi} \int \frac{1}{|x-y|} |U_{\beta, \beta_1}(y)| d^2y$$

separately. Let first $2RN^{-\beta} \leq |x|$. Similarly as in the previous argument, one finds

$$\int \frac{1}{|x-y|} |W_\beta(y)| d^2y \leq \int_{B_{RN^{-\beta}(0)}} \frac{1}{|x-y|} |W_\beta(y)| d^2y \leq \frac{\|W_\beta\|_1}{|x| - RN^{-\beta}}$$

for $RN^{-\beta} \leq |x|$, which implies that

$$\int \frac{1}{|x-y|} |W_\beta(y)| d^2y \leq \frac{C \|W_\beta\|_1}{(|x|^2 + N^{-2\beta})^{\frac{1}{2}}} \leq \frac{CN^{-1}}{(|x|^2 + N^{-2\beta})^{\frac{1}{2}}}$$

for all $2RN^{-\beta} \leq |x|$. For $|x| \leq 2RN^{-\beta}$, we make use of

$$N^\beta \leq \frac{C}{(|x|^2 + N^{-2\beta})^{1/2}}$$

and estimate

$$\begin{aligned} \int \frac{1}{|x-y|} |W_\beta(y)| d^2y &\leq \|W_\beta\|_\infty \int_{B_{RN^{-\beta}(0)}} \frac{1}{|x-y|} d^2y \\ &\leq CN^{2\beta-1} \int_0^{RN^{-\beta}} dr = CN^{-1+\beta} \leq \frac{CN^{-1}}{(|x|^2 + N^{-2\beta})^{1/2}}. \end{aligned}$$

Equivalently, we obtain

$$\begin{aligned} \int \frac{1}{|x-y|} U_{\beta_1, \beta}(y) d^2y &\leq \|U_{\beta_1, \beta}\|_\infty \int_{B_{N^{-\beta_1}(0)}} \frac{1}{|x-y|} d^2y \\ &= CN^{-1+\beta_1} \leq \frac{CN^{-1}}{(|x|^2 + N^{-2\beta_1})^{1/2}} \leq \frac{CN^{-1}}{(|x|^2 + N^{-2\beta})^{\frac{1}{2}}}, \end{aligned}$$

for $|x| \leq N^{-\beta_1}$. Since $\nabla h_{\beta_1, \beta}(x) = 0$ for $|x| \geq N^{-\beta_1}$, the second statement of (b) follows.

(c) The first part of (c) follows from (b) and the fact that the support of $h_{\beta_1, \beta}$ and $\nabla h_{\beta_1, \beta}$ has radius $\leq CN^{-\beta_1}$. The bounds on the L^2 -norm can be improved by

$$\begin{aligned} \|\nabla h_{\beta_1, \beta}\|^2 &\leq C \int_0^{CN^{-\beta_1}} dr r |\nabla h_{\beta_1, \beta}(r)|^2 \leq \frac{C}{N^2} \int_0^{CN^{-\beta_1}} dr \frac{r}{r^2 + N^{-2\beta}} \\ &= \frac{C}{N^2} \ln \left(\frac{N^{-2\beta_1} + N^{-2\beta}}{N^{-2\beta}} \right) \leq \frac{C}{N^2} \ln(N). \end{aligned}$$

Using, for $|x| \geq 2RN^{-\beta}$, the inequality

$$|h_{0, \beta}(x)| \leq CN^{-1} |\ln(|x| - RN^{-\beta})|,$$

we obtain

$$\begin{aligned} \|h_{0, \beta}\|_2^2 &= \int_{\mathbb{R}^2} d^2x \mathbb{1}_{B_{2RN^{-\beta}(0)}}(x) |h_{0, \beta}(x)|^2 + \int_{\mathbb{R}^2} d^2x \mathbb{1}_{B_{2RN^{-\beta}(0)}^c}(x) |h_{0, \beta}(x)|^2 \\ &\leq \|h_{0, \beta}\|_\infty^2 |B_{2RN^{-\beta}(0)}| + CN^{-2} \int_{2RN^{-\beta}}^1 dr r |\ln(r - RN^{-\beta})|^2 \\ &\leq C \left(N^{-2-2\beta} (\ln(N))^2 + N^{-2} \int_{RN^{-\beta}}^1 dr (r + RN^{-\beta}) (\ln(r))^2 \right). \end{aligned}$$

Using

$$\begin{aligned}
& \int_{RN^{-\beta}}^1 dr (r + RN^{-\beta}) (\ln(r))^2 \\
&= \left(\frac{1}{4} r^2 (2(\ln(r))^2 - 2\ln(r) + 1) + RN^{-\beta} r ((\ln(r))^2 - 2\ln(r) + 2) \right) \Big|_{RN^{-\beta}}^1 \\
&\leq C (1 + N^{-\beta} + N^{-2\beta} (\ln(N))^2),
\end{aligned}$$

we obtain, for any $\beta > 0$,

$$\|h_{0,\beta}\|_2^2 \leq CN^{-2} (1 + N^{-\beta} + N^{-2\beta} (\ln(N))^2) \leq CN^{-2}.$$

□

3.5.3 Estimates on the cutoff

In the previous Lemma we defined an auxiliary potential $U_{\beta_1, \beta}$ and sketched the idea how one can employ this potential to obtain sufficient bounds. We will use this strategy to estimate the Contributions (3.30) and (3.31). One would therefore like to control the quantity $\|\nabla_1 q_1 \Psi_t\|$ sufficiently well to show convergence of the reduced density matrices. While it is indeed possible to obtain a sufficient bound of $\|\nabla_1 q_1 \Psi_t\|$ in the case where the dynamics is generated by the Hamiltonian H_{W_β} , this term will in fact not be small for the dynamic generated by H_{V_N} . Due to the presence of the short-scale correlation structure, we then rather expect $\|\nabla_1 q_1 \Psi_t\| = \mathcal{O}(1)$ to hold. This presumption has been shown in [15] and [39] in the static case. In particular, the results of these papers show that the interaction energy is purely kinetic in the Gross-Pitaevskii regime, which implies that a relevant part of the kinetic energy is concentrated around the scattering centers. We must thus separate the part which is used to form the microscopic structure. For this, we define the set $\overline{\mathcal{A}}_j^{(d)}$ which includes all configurations where the distance between particle x_i and particle $x_j, j \neq i$ is smaller than N^{-d} . It is then possible to prove that the kinetic energy concentrated on the complement of $\overline{\mathcal{A}}_j^{(d)}$, i.e. $\|\mathbb{1}_{\mathcal{A}_j^{(d)}} \nabla_1 q_1 \Psi\|$, can be controlled sufficiently well, see Lemma 3.5.10. Next, we provide several bounds which will be used to incorporate this idea in a rigorous manner.

Definition 3.5.4 For any $j, k = 1, \dots, N$ and $d > 0$ let

$$a_{j,k}^{(d)} = \{(x_1, x_2, \dots, x_N) \in \mathbb{R}^{2N} : |x_j - x_k| < N^{-d}\} \subseteq \mathbb{R}^{2N}, \quad (3.48)$$

$$\overline{\mathcal{A}}_j^{(d)} = \bigcup_{k \neq j} a_{j,k}^{(d)} \quad \mathcal{A}_j^{(d)} = \mathbb{R}^{2N} \setminus \overline{\mathcal{A}}_j^{(d)} \quad \overline{\mathcal{B}}_j^{(d)} = \bigcup_{k \neq l \neq j} a_{k,l}^{(d)} \quad \mathcal{B}_j^{(d)} = \mathbb{R}^{2N} \setminus \overline{\mathcal{B}}_j^{(d)}.$$

Lemma 3.5.5 Let $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap H^1(\mathbb{R}^{2N}, \mathbb{C})$ $\|\Psi\| = 1$ and let $\|\nabla_1 \Psi\|$ be uniformly bounded in N . Then, for all $j \neq k$ with $1 \leq j, k \leq N$,

(a)

$$\begin{aligned}\|\mathbb{1}_{\overline{\mathcal{A}}_j^{(d)}} p_j\|_{op} &\leq C\|\varphi\|_\infty N^{1/2-d}, \\ \|\mathbb{1}_{\overline{\mathcal{A}}_j^{(d)}} \nabla_j p_j\|_{op} &\leq C\|\nabla\varphi\|_\infty N^{1/2-d}, \\ \|\mathbb{1}_{a_{j,k}^{(d)}} p_j\|_{op} &\leq C\|\varphi\|_\infty N^{-d}.\end{aligned}$$

(b) For any $\epsilon > 0$, there exists a constant C_ϵ , such that

$$\|\mathbb{1}_{\overline{\mathcal{A}}_j^{(d)}} \Psi\| \leq C_\epsilon N^{\frac{1}{2}-d+\epsilon}. \quad (3.49)$$

(c) For any $\epsilon > 0$, there exists a constant $C_\epsilon > 0$, such that

$$\|\mathbb{1}_{\overline{\mathcal{B}}_j^{(d)}} \Psi\| \leq C_\epsilon N^{1-d+\epsilon} \quad (3.50)$$

holds.

(d) For any $k \neq j$

$$\|[\mathbb{1}_{\overline{\mathcal{A}}_j^{(d)}}, p_k]\|_{op} = \|[\mathbb{1}_{a_{j,k}^{(d)}}, p_k]\|_{op} = \|[\mathbb{1}_{\overline{\mathcal{A}}_j^{(d)}}, p_k]\|_{op} \leq C\|\varphi\|_\infty N^{-d}.$$

Proof:

(a) First note that the volume of the sets $a_{j,k}^{(d)}$ introduced in Definition 3.5.4 are $|a_{j,k}^{(d)}| = \pi N^{-2d}$.

$$\|\mathbb{1}_{\overline{\mathcal{A}}_j^{(d)}} p_j\|_{op} = \|\mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} p_1\|_{op} = \|p_1 \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} p_1\|_{op}^{\frac{1}{2}} \leq \left(\|\varphi\|_\infty^2 \|\mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}}\|_{1,\infty}\right)^{1/2}$$

where we defined

$$\|f\|_{p,\infty} = \sup_{x_2, \dots, x_N \in \mathbb{R}^2} \left(\int dx_1 |f(x_1, \dots, x_N)|^p \right)^{\frac{1}{p}}.$$

Using $\mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \leq \sum_{k=2}^N \mathbb{1}_{a_{1,k}^{(d)}}$ as well as $\left(\mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}}\right)^p = \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}}$, we obtain

$$\|\mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}}\|_{p,\infty} \leq \sup_{x_2, \dots, x_N \in \mathbb{R}^2} \left(\int dx_1 \sum_{k=2}^N \mathbb{1}_{a_{1,k}^{(d)}} \right)^{\frac{1}{p}} \leq (N|a_{1,k}|)^{\frac{1}{p}} \leq CN^{(1-2d)\frac{1}{p}}.$$

This implies

$$\|\mathbb{1}_{\overline{\mathcal{A}}_j^{(d)}} p_j\|_{op} \leq C\|\varphi\|_\infty N^{\frac{1}{2}-d}.$$

The second statement of (a) can be proven similarly. Analogously, we obtain

$$\|\mathbb{1}_{a_{j,k}^{(d)}} p_j\|_{op} \leq \|\varphi\|_\infty |a_{j,k}^{(d)}|^{1/2} \leq C\|\varphi\|_\infty N^{-d}$$

(b) Without loss of generality, we can set $j = 1$. Recall the two-dimensional Sobolev inequality (also called Gagliardo-Nirenberg interpolation inequality): For any $\varrho \in H^1(\mathbb{R}^2, \mathbb{C})$ and for any $2 < m < \infty$, there exists a constant C_m , depending only on m , such that $\|\varrho\|_m \leq C_m \|\nabla \varrho\|^{\frac{m-2}{m}} \|\varrho\|^{\frac{2}{m}}$ holds. Using Hölder and Sobolev for the x_1 -integration, we get, for $p > 1$

$$\begin{aligned} \|\mathbf{1}_{\overline{\mathcal{A}}_1^{(d)}} \Psi\|^2 &= \langle \Psi, \mathbf{1}_{\overline{\mathcal{A}}_1^{(d)}} \Psi \rangle = \int d^2 x_2 \dots d^2 x_N \int d^2 x_1 |\Psi(x_1, \dots, x_N)|^2 \mathbf{1}_{\overline{\mathcal{A}}_1^{(d)}}(x_1, \dots, x_N) \\ &\leq \|\mathbf{1}_{\overline{\mathcal{A}}_1^{(d)}}\|_{\frac{p}{p-1}, \infty} \int d^2 x_2 \dots d^2 x_N \left(\int d^2 x_1 |\Psi(x_1, \dots, x_N)|^{2p} \right)^{1/p} \\ &\leq C_p N^{(1-2d)\frac{p-1}{p}} \int d^2 x_2 \dots d^2 x_N \left(\int d^2 x_1 |\nabla_1 \Psi(x_1, \dots, x_N)|^2 \right)^{\frac{p-1}{p}} \left(\int d^2 \tilde{x}_1 |\Psi(\tilde{x}_1, \dots, x_N)|^2 \right)^{\frac{1}{p}}. \end{aligned}$$

Using Hölder for the x_2, \dots, x_N -integration with the conjugate pair $r = \frac{p}{p-1}$ and $s = p$, we obtain

$$\|\mathbf{1}_{\overline{\mathcal{A}}_1^{(d)}} \Psi\|^2 \leq C_p N^{(1-2d)\frac{p-1}{p}} \|\nabla_1 \Psi\|^{2\frac{p-1}{p}} \|\Psi\|^{\frac{2}{p}}.$$

Using $\|\nabla_1 \Psi\| < C$, (b) follows.

(c) We use that $\overline{\mathcal{B}}_j^{(d)} \subset \bigcup_{k=1}^N \overline{\mathcal{A}}_k^{(d)}$. Hence one can find pairwise disjoint sets $\mathcal{C}_k \subset \overline{\mathcal{A}}_k^{(d)}$, $k = 1, \dots, N$ such that $\overline{\mathcal{B}}_j^{(d)} \subset \bigcup_{k=1}^N \mathcal{C}_k$. Since the sets \mathcal{C}_k are pairwise disjoint, the wavefunctions $\mathbf{1}_{\mathcal{C}_k} \Psi$ are pairwise orthogonal and we get

$$\|\mathbf{1}_{\overline{\mathcal{B}}_j^{(d)}} \Psi\|^2 \leq \sum_{k=1}^N \|\mathbf{1}_{\mathcal{C}_k} \Psi\|^2 \leq \sum_{k=1}^N \|\mathbf{1}_{\overline{\mathcal{A}}_k^{(d)}} \Psi\|^2.$$

(d)

$$\begin{aligned} \|\mathbf{1}_{\overline{\mathcal{A}}_1^{(d)}} \Psi\|_{\text{op}} &\leq \|\mathbf{1}_{a_{1,2}} \Psi\|_{\text{op}} \leq \|\mathbf{1}_{a_{1,2}} p_2\|_{\text{op}} + \|p_2 \mathbf{1}_{a_{1,2}}\|_{\text{op}} \\ &\leq 2\|\varphi\|_{\infty} |a_{1,2}|^{\frac{1}{2}} \leq C\|\varphi\|_{\infty} N^{-d}. \end{aligned}$$

□

3.5.4 Estimates for the functionals γ_a , $\gamma_a^<$ and $\gamma_b^<$

Control of γ_a and $\gamma_a^<$ The next well-known Lemma, which can e.g. be found on p.30 in [60], can be applied readily to estimate $\gamma_a, \gamma_a^<$.

Lemma 3.5.6 *For any multiplication operator $B : L^2(\mathbb{R}^2, \mathbb{C}) \rightarrow L^2(\mathbb{R}^2, \mathbb{C})$ and any $\varphi \in L^2(\mathbb{R}^2, \mathbb{C})$ and any $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C})$ we have*

$$|\langle \Psi, B(x_1) \Psi \rangle - \langle \varphi, B\varphi \rangle| \leq C\|B\|_{\infty} (\langle \Psi, \widehat{n}^{\varphi} \Psi \rangle + N^{-\frac{1}{2}}).$$

Proof: Using $1 = p_1 + q_1$,

$$\begin{aligned}
& \langle\langle \Psi, B(x_1)\Psi \rangle\rangle - \langle \varphi, B\varphi \rangle \\
&= \langle\langle \Psi, p_1 B(x_1)p_1 \Psi \rangle\rangle + 2\Re \langle\langle \Psi, q_1 B(x_1)p_1 \Psi \rangle\rangle + \langle\langle \Psi, q_1 B(x_1)q_1 \Psi \rangle\rangle - \langle \varphi, B\varphi \rangle \\
&\leq \langle \varphi, B\varphi \rangle (\|p_1 \Psi\|^2 - 1) + 2\Re \langle\langle \Psi, \widehat{n}^{-1/2} q_1 B(x_1)p_1 \widehat{n}_1^{1/2} \Psi \rangle\rangle \\
&\quad + \langle\langle \Psi, q_1 B(x_1)q_1 \Psi \rangle\rangle
\end{aligned}$$

where we used Lemma 2.0.5 (c). Since $\|p_1 \Psi\|^2 - 1 = \|q_1 \Psi\|^2$ it follows that

$$\begin{aligned}
|\langle\langle \Psi, B(x_1)\Psi \rangle\rangle - \langle \varphi, B\varphi \rangle| &\leq C\|B\|_\infty (\langle\langle \Psi, \widehat{n}^2 \Psi \rangle\rangle + \langle\langle \Psi, \widehat{n}_1 \Psi \rangle\rangle + \langle\langle \Psi, \widehat{n} \Psi \rangle\rangle) \\
&\leq C\|B\|_\infty (\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + N^{-\frac{1}{2}}).
\end{aligned} \tag{3.51}$$

□

Using Lemma 3.5.6, setting $B = \dot{A}_t$, we get

$$\gamma_a^<(\Psi_t, \varphi_t) = \gamma_a(\Psi_t, \varphi_t) \leq C\|\dot{A}_t\|_\infty (\langle\langle \Psi_t, \widehat{n}^{\varphi_t} \Psi_t \rangle\rangle + N^{-\frac{1}{2}}),$$

which yields the first Bound (3.33) in Lemma 3.4.6.

Control of $\gamma_b^<$ To control $\gamma_b^<$, we first derive some bounds on the operator norms associated with the counting measures \widehat{m}^a and \widehat{m}^b , which were defined in Definition 3.4.2. The difference $m(k) - m(k+1)$ and $m(k) - m(k+2)$ is approximately given by the derivative of $m(k)$ w.r.t. k , which equals

$$m(k)' = \begin{cases} 1/(2\sqrt{kN}), & \text{for } k \geq N^{1-2\xi}; \\ 1/2(N^{-1+\xi}), & \text{else.} \end{cases} \tag{3.52}$$

It is then easy to verify that, for any $j \in \mathbb{Z}$, there exists a $C_j < \infty$ such that

$$\widehat{m}_j^x \leq C_j N^{-1} \widehat{n}^{-1} \text{ for } x \in \{a, b\} \tag{3.53}$$

$$\|\widehat{m}_j^x\|_{\text{op}} \leq C_j N^{-1+\xi} \text{ for } x \in \{a, b\} \tag{3.54}$$

$$\|\widehat{n}\widehat{m}_j^x\|_{\text{op}} \leq C_j N^{-1} \text{ for } x \in \{a, b\} \tag{3.55}$$

$$\|\widehat{r}\|_{\text{op}} \leq \|\widehat{m}^a\|_{\text{op}} + \|\widehat{m}^b\|_{\text{op}} \leq C N^{-1+\xi}. \tag{3.56}$$

The different terms we have to estimate for $\gamma_b^<$ can be found in Eq. (3.29). In order to facilitate the notation, let $\widehat{w} \in \{N\widehat{m}_{-1}^a, N\widehat{m}_{-2}^b\}$. Then $w(k) < n(k)^{-1}$ and $\|\widehat{w}\|_{\text{op}} \leq C N^\xi$ follows.

Lemma 3.5.7 *Let $\beta > 0$ and $W_\beta \in \mathcal{V}_\beta$ as in Definition 3.3.4. Let $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap H^2(\mathbb{R}^{2N}, \mathbb{C})$, $\|\Psi\| = 1$ and let $\|\nabla_1 \Psi\| \leq \mathcal{K}(\varphi, A)$. Let $w(k) < n(k)^{-1}$ and $\|\widehat{w}\|_{\text{op}} \leq C N^\xi$ for some $\xi \geq 0$. Then,*

(a)

$$N \left| \langle\langle \Psi p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 p_2 \widehat{w} \Psi \rangle\rangle \right| \leq \mathcal{K}(\varphi, A) (N^{-1} + N^{-2\beta} \ln(N)).$$

(b)

$$N|\langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) \widehat{w} q_1 q_2 \Psi \rangle\rangle| \leq \mathcal{K}(\varphi, A.) \left(\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + \inf_{\eta > 0} \inf_{\beta_1 > 0} (N^{\eta-2\beta_1} \ln(N)^2 + \|\widehat{w}\|_{op} N^{-1+2\beta_1} + \|\widehat{w}\|_{op}^2 N^{-\eta}) \right).$$

(c)

$$N|\langle\langle \Psi p_1 q_2 Z_\beta^\varphi(x_1, x_2) \widehat{w} q_1 q_2 \Psi \rangle\rangle| \leq \mathcal{K}(\varphi, A.) \left(\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + N^{-1/6} \ln(N) + \inf \left\{ |\mathcal{E}_{V_N}(\Psi) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi)|, |\mathcal{E}_{W_\beta}(\Psi) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi)| + N^{-2\beta} \ln(N) \right\} \right).$$

Proof:

(a) In view of Lemma 2.0.7, we obtain

$$N|\langle\langle \Psi, p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 p_2 \widehat{w} \Psi \rangle\rangle| \leq N \|p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 p_2\|_{op} \|\widehat{n} \widehat{w} \Psi\| \leq C N \|p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 p_2\|_{op}.$$

$\|p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 p_2\|_{op}$ can be estimated using $p_1 q_1 = 0$ and (2.7):

$$\begin{aligned} & N \left\| p_1 p_2 \left(W_\beta(x_1 - x_2) - \frac{b_{W_\beta}}{N-1} |\varphi(x_1)|^2 - \frac{b_{W_\beta}}{N-1} |\varphi(x_2)|^2 \right) q_1 p_2 \right\|_{op} \\ & \leq \|p_1 p_2 (N W_\beta(x_1 - x_2) - b_{W_\beta} d^2 x |\varphi(x_1)|^2) p_2\|_{op} + C \|\varphi\|_\infty^2 N^{-1} \\ & \leq \|\varphi\|_\infty \|N (W_\beta \star |\varphi|^2) - N \int_{\mathbb{R}^2} W_\beta(x) d^2 x |\varphi|^2\| + C \|\varphi\|_\infty^2 N^{-1}. \end{aligned}$$

Let h be given by

$$h(x) = -\frac{1}{2\pi} \int_{\mathbb{R}^2} d^2 y \ln|x - y| N W_\beta(y) + \frac{1}{2\pi} b_{W_\beta} \ln|x|,$$

which implies

$$\Delta h(x) = N W_\beta(x) - b_{W_\beta} \delta(x).$$

As above (see Lemma 3.5.3), we obtain $h(x) = 0$ for $x \notin B_{RN^{-\beta}}(0)$, where $R N^{-\beta}$ is the radius of the support of W_β .

Thus,

$$\|h\|_1 \leq \frac{1}{2\pi} \int_{\mathbb{R}^2} d^2 x \int_{\mathbb{R}^2} d^2 y |\ln|x - y|| \mathbb{1}_{B_{RN^{-\beta}}(0)}(x) N W_\beta(y) \quad (3.57)$$

$$- \frac{1}{2\pi} b_{W_\beta} \int_{\mathbb{R}^2} d^2 x \ln(|x|) \mathbb{1}_{B_{RN^{-\beta}}(0)}(x) \leq C N^{-2\beta} \ln(N). \quad (3.58)$$

We integrate by parts twice and use Young's inequality to obtain

$$\begin{aligned} \|N(W_\beta \star |\varphi|^2) - b_{W_\beta} |\varphi|^2\| &= \|(\Delta h) \star |\varphi|^2\| \\ &\leq \|h\|_1 \|\Delta |\varphi|^2\|_2 \leq \mathcal{K}(\varphi, A.) N^{-2\beta} \ln(N). \end{aligned}$$

Thus, we obtain the bound

$$N |\langle\langle \Psi, p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 p_2 \widehat{w} \Psi \rangle\rangle| \leq \mathcal{K}(\varphi, A.) (N^{-1} + N^{-2\beta} \ln(N)), \quad (3.59)$$

which then proves part (a).

(b) We will first consider $\beta < 1/2$.

With Lemma 2.0.5 (c) and Lemma 2.0.10 with

$$\begin{aligned} O_{1,2} &= q_2 W_\beta(x_1 - x_2) p_2, \quad \Omega = N^{-1/2} (\widehat{w})^{1/2} q_1 \Psi \\ \chi &= N^{1/2} p_1 (\widehat{w}_2)^{1/2} \Psi, \end{aligned}$$

we obtain the bound

$$\begin{aligned} &|\langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \widehat{w} \Psi \rangle\rangle| \\ &= |\langle\langle \Psi, (\widehat{w})^{1/2} q_1 q_2 W_\beta(x_1 - x_2) p_1 p_2 (\widehat{w}_2)^{1/2} \Psi \rangle\rangle| \\ &\leq N^{-1} \|(\widehat{w})^{1/2} q_1 \Psi\|^2 + N |\langle\langle q_2 (\widehat{w}_2)^{1/2} \Psi, p_1 \sqrt{|W_\beta(x_1 - x_2)|} p_3 \sqrt{|W_\beta(x_1 - x_3)|} \\ &\quad \sqrt{|W_\beta(x_1 - x_2)|} p_2 \sqrt{|W_\beta(x_1 - x_3)|} p_1 q_3 (\widehat{w}_2)^{1/2} \Psi \rangle\rangle| \\ &\quad + N(N-1)^{-1} \|q_2 W_\beta(x_1 - x_2) p_2 p_1 (\widehat{w}_2)^{1/2} \Psi\|^2 \\ &\leq N^{-1} \|(\widehat{w})^{1/2} q_1 \Psi\|^2 + N \|\sqrt{|W_\beta(x_1 - x_2)|} p_1\|_{\text{op}}^4 \|q_2 (\widehat{w}_2)^{1/2} \Psi\|^2 \\ &\quad + 2N(N-1)^{-1} \|p_1 q_2 (\widehat{w}_1)^{1/2} W_\beta(x_1 - x_2) p_2 p_1 \Psi\|^2 \\ &\quad + 2N(N-1)^{-1} \|q_1 q_2 (\widehat{w})^{1/2} W_\beta(x_1 - x_2) p_2 p_1 \Psi\|^2. \end{aligned}$$

Lemma 2.0.5 (e) then yields

$$\begin{aligned} |\langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \widehat{w} \Psi \rangle\rangle| &\leq N^{-1} \|(\widehat{w})^{1/2} \widehat{n} \Psi\|^2 + N \|\varphi\|_\infty^4 \|W_\beta\|_1^2 \|\widehat{n} (\widehat{w}_2)^{1/2} \Psi\|^2 \\ &\quad + 2N(N-1)^{-1} \|W_\beta\|^2 \|\varphi\|_\infty^2 (\|\widehat{w}_1\|_{\text{op}} + \|\widehat{w}\|_{\text{op}}). \end{aligned}$$

Note, that $\|W_\beta\|_1 \leq CN^{-1}$, $\|W_\beta\|^2 \leq CN^{-2+2\beta}$. Furthermore, using $\widehat{n} < \widehat{n}_2$, we have under the conditions on \widehat{w}

$$\|(\widehat{w})^{1/2} \widehat{n}_2 \Psi\| \leq \|(\widehat{w}_2)^{1/2} \widehat{n}_2 \Psi\| \leq \|(\widehat{n}_2)^{1/2} \Psi\| \leq \sqrt{\langle \Psi, \widehat{n} \Psi \rangle} + 2N^{-\frac{1}{2}}. \quad (3.60)$$

In total, we obtain

$$N |\langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \widehat{w} \Psi \rangle\rangle| \leq \mathcal{K}(\varphi, A.) (\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + \|\widehat{w}\|_{\text{op}} N^{-1+2\beta})$$

and we get (b) for the case $\beta < 1/2$.

(b) for $1/2 \leq \beta$: We use $U_{\beta_1, \beta}$ from Definition 3.5.2 for some $0 < \beta_1 < 1/2$. We then obtain

$$\begin{aligned} & N \langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) \widehat{w} q_1 q_2 \Psi \rangle\rangle \\ &= N \langle\langle \Psi, p_1 p_2 U_{\beta_1, \beta}(x_1 - x_2) \widehat{w} q_1 q_2 \Psi \rangle\rangle \end{aligned} \quad (3.61)$$

$$+ N \langle\langle \Psi, p_1 p_2 (W_\beta(x_1 - x_2) - U_{\beta_1, \beta}(x_1 - x_2)) \widehat{w} q_1 q_2 \Psi \rangle\rangle. \quad (3.62)$$

Term (3.61) has been controlled above. So we are left to control (3.62).

Let $\Delta h_{\beta_1, \beta} = W_\beta - U_{\beta_1, \beta}$. Integrating by parts and using that

$\nabla_1 h_{\beta_1, \beta}(x_1 - x_2) = -\nabla_2 h_{\beta_1, \beta}(x_1 - x_2)$ gives

$$\begin{aligned} & N |\langle\langle \Psi, p_1 p_2 (W_\beta(x_1 - x_2) - U_{\beta_1, \beta}(x_1 - x_2)) \widehat{w} q_1 q_2 \Psi \rangle\rangle| \\ & \leq N |\langle\langle \nabla_1 p_1 \Psi, p_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) \widehat{w} q_1 q_2 \Psi \rangle\rangle| \end{aligned} \quad (3.63)$$

$$+ N |\langle\langle \Psi, p_1 p_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) \nabla_1 \widehat{w} q_1 q_2 \Psi \rangle\rangle|. \quad (3.64)$$

Let $t_1 \in \{p_1, \nabla_1 p_1\}$ and let $\Gamma \in \{\widehat{w} q_1 \Psi, \nabla_1 \widehat{w} q_1 \Psi\}$.

For both (3.63) and (3.64), we use Lemma 2.0.10 with

$$O_{1,2} = N^{1+\eta/2} q_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) p_2, \quad \chi = t_1 \Psi, \quad \Omega = N^{-\eta/2} \Gamma.$$

This yields

$$(3.63) + (3.64) \leq 2 \sup_{t_1 \in \{p_1, \nabla_1 p_1\}, \Gamma \in \{\widehat{w} q_1 \Psi, \nabla_1 \widehat{w} q_1 \Psi\}} \left(N^{-\eta} \|\Gamma\|^2 \right) \quad (3.65)$$

$$+ \frac{N^{2+\eta}}{N-1} \|q_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) t_1 p_2 \Psi\|^2 \quad (3.66)$$

$$+ N^{2+\eta} |\langle\langle \Psi, t_1 p_2 q_3 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) \nabla_3 h_{\beta_1, \beta}(x_1 - x_3) t_1 q_2 p_3 \Psi \rangle\rangle|. \quad (3.67)$$

The first term can be bounded using Corollary 2.0.8 by

$$\begin{aligned} N^{-\eta} \|\nabla_1 \widehat{w} q_1 \Psi\|^2 &\leq N^{-\eta} \|\widehat{w}\|_{\text{op}}^2 \|\nabla_1 q_1 \Psi\|^2 \\ N^{-\eta} \|\widehat{w} q_1 \Psi\|^2 &\leq C N^{-\eta}. \end{aligned}$$

Thus (3.65) $\leq \mathcal{K}(\varphi, A.) N^{-\eta} \|\widehat{w}\|_{\text{op}}^2$ using that $\|\nabla_1 q_1 \Psi\| \leq \mathcal{K}(\varphi, A.)$. By $\|t_1 \Psi\|^2 \leq \mathcal{K}(\varphi, A.)$, we obtain

$$\begin{aligned} (3.66) &\leq \mathcal{K}(\varphi, A.) \frac{N^{2+\eta}}{N-1} \|\nabla_2 h_{\beta_1, \beta}(x_1 - x_2) p_2\|_{\text{op}}^2 \leq \mathcal{K}(\varphi, A.) \frac{N^{2+\eta}}{N-1} \|\varphi\|_\infty^2 \|\nabla h_{\beta_1, \beta}\|^2 \\ &\leq \mathcal{K}(\varphi, A.) N^{\eta-1} \ln(N), \end{aligned}$$

where we used Lemma 3.5.3 in the last step.

Next, we estimate

$$\begin{aligned}
(3.67) \leq & N^{2+\eta} \|p_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) t_1 q_2 \Psi\|^2 \\
\leq & 2N^{2+\eta} \|p_2 h_{\beta_1, \beta}(x_1 - x_2) t_1 \nabla_2 q_2 \Psi\|^2 \\
& + 2N^{2+\eta} \|\langle \varphi(x_2) \rangle \langle \nabla \varphi(x_2) | h_{\beta_1, \beta}(x_1 - x_2) t_1 q_2 \Psi \rangle\|^2 \\
\leq & 2N^{2+\eta} \|p_2 h_{\beta_1, \beta}(x_1 - x_2)\|_{\text{op}}^2 \|t_1 \nabla_2 q_2 \Psi\|^2 \\
& + 2N^{2+\eta} \|\langle \varphi(x_2) \rangle \langle \nabla \varphi(x_2) | h_{\beta_1, \beta}(x_1 - x_2)\|_{\text{op}}^2 \|t_1 q_2 \Psi\|^2 \\
\leq & \mathcal{K}(\varphi, A.) N^{2+\eta} \|h_{\beta_1, \beta}\|^2 \\
\leq & \mathcal{K}(\varphi, A.) N^{\eta-2\beta_1} \ln(N)^2.
\end{aligned}$$

Thus, for all $\eta \in \mathbb{R}$

$$\begin{aligned}
& N \langle\langle \Psi, p_1 p_2 (W_\beta(x_1 - x_2) - U_{\beta_1, \beta}(x_1 - x_2)) \widehat{w} q_1 q_2 \Psi \rangle\rangle \\
& \leq \mathcal{K}(\varphi, A.) (\|\widehat{w}\|_{\text{op}}^2 N^{-\eta} + N^{\eta-1} \ln(N) + N^{\eta-2\beta_1} \ln(N)^2).
\end{aligned}$$

Combining both estimates for $\beta < 1/2$ and $\beta \geq 1/2$, we obtain, using $N^{\eta-1} \ln(N) < N^{\eta-2\beta_1} \ln(N)$,

$$\begin{aligned}
& N \langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) \widehat{w} q_1 q_2 \Psi \rangle\rangle \tag{3.68} \\
& \leq \mathcal{K}(\varphi, A.) \left(\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + \inf_{\eta > 0} \inf_{\beta_1 > 0} (N^{\eta-2\beta_1} \ln(N)^2 + N^{-1+2\beta_1} + \|\widehat{w}\|_{\text{op}}^2 N^{-\eta}) \right).
\end{aligned}$$

and we get (b) in full generality.

(c) We first estimate, noting that $q_1 p_2 |\varphi|^2(x_1) q_1 q_2 = 0$,

$$\begin{aligned}
& N \left| \langle\langle \Psi, q_1 p_2 \frac{b_{W_\beta}}{N-1} |\varphi|^2(x_2) \widehat{w} q_1 q_2 \Psi \rangle\rangle \right| \leq C \|\varphi\|_\infty^2 \|\widehat{w} q_1 q_2 \Psi\| \|q_1 \Psi\| \\
& \leq C \|\varphi\|_\infty^2 \|\widehat{w} \widehat{n}^2 \Psi\| \|q_1 \Psi\| \leq \mathcal{K}(\varphi, A.) \langle\langle \Psi, \widehat{n} \Psi \rangle\rangle.
\end{aligned}$$

It is left to estimate $N |\langle\langle \Psi, q_1 p_2 W_\beta(x_1 - x_2) \widehat{w} q_1 q_2 \Psi \rangle\rangle|$. Let $U_{0, \beta}$ be given as in Definition 3.5.2.

Using Lemma 2.0.5 (c) and integrating by parts we get

$$\begin{aligned}
& N |\langle \Psi, q_1 p_2 W_\beta(x_1 - x_2) \widehat{w} q_1 q_2 \Psi \rangle| \\
& \leq N |\langle \Psi, q_1 p_2 U_{0,\beta}(x_1 - x_2) q_1 q_2 \widehat{w} \Psi \rangle| + N |\langle \Psi, q_1 p_2 (\Delta_1 h_{0,\beta}(x_1 - x_2)) q_1 q_2 \widehat{w} \Psi \rangle| \\
& \leq \|U_{0,\beta}\|_\infty N \|q_1 \Psi\| \|\widehat{w} q_1 q_2 \Psi\| \\
& + N |\langle \nabla_1 q_1 p_2 \Psi, (\nabla_1 h_{0,\beta}(x_1 - x_2)) \widehat{w} q_1 q_2 \Psi \rangle| \\
& + N |\langle \Psi, \widehat{w}_1 q_1 p_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) \nabla_1 q_1 q_2 \Psi \rangle| \\
& \leq N \|U_{0,\beta}\|_\infty \|q_1 \Psi\| \|\widehat{w} q_1 q_2 \Psi\| \tag{3.69}
\end{aligned}$$

$$+ N \left| \langle \mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi, p_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) \widehat{w} q_1 q_2 \Psi \rangle \right| \tag{3.70}$$

$$+ N \left| \langle \nabla_1 q_1 \Psi, \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} p_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) q_1 q_2 \widehat{w} \Psi \rangle \right| \tag{3.71}$$

$$+ N \left| \langle \Psi, \widehat{w}_1 q_1 p_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) q_2 \mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi \rangle \right| \tag{3.72}$$

$$+ N \left| \langle \Psi, \widehat{w}_1 q_1 p_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) q_2 \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 q_1 \Psi \rangle \right|. \tag{3.73}$$

Lemma 2.0.7 and Lemma 3.5.3 (a) yields the bound

$$(3.69) \leq C \langle \Psi, \widehat{n} \Psi \rangle.$$

For (3.71) and (3.73) we use Cauchy Schwarz and then Sobolev inequality as in Lemma 3.5.5 to get, for any $p > 1$,

$$\begin{aligned}
(3.71) + (3.73) & \leq N \|\nabla_1 q_1 \Psi\| \left\| \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} p_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) q_1 q_2 \widehat{w} \Psi \right\| \\
& + N \|\nabla_1 q_1 \Psi\| \left\| \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} q_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) q_1 p_2 \widehat{w}_1 \Psi \right\| \\
& \leq C_p N \|\nabla_1 q_1 \Psi\| N^{\frac{1-2d}{2} \frac{p-1}{p}} \|\nabla_1 p_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) q_1 q_2 \widehat{w} \Psi\|^{\frac{p-1}{p}} \\
& \times \|p_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) q_1 q_2 \widehat{w} \Psi\|^{1/p} \\
& + C_p N \|\nabla_1 q_1 \Psi\| N^{\frac{1-2d}{2} \frac{p-1}{p}} \|\nabla_1 q_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) q_1 p_2 \widehat{w}_1 \Psi\|^{\frac{p-1}{p}} \\
& \times \|q_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) q_1 p_2 \widehat{w}_1 \Psi\|^{1/p}.
\end{aligned}$$

Using Lemma 2.0.5, Lemma 2.0.7, Corollary 2.0.8 and Lemma 3.5.3, we obtain

$$\begin{aligned}
& \|\nabla_1 p_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) q_1 q_2 \widehat{w} \Psi\| \leq \|p_2 (\Delta_1 h_{0,\beta}(x_1 - x_2)) q_1 q_2 \widehat{w} \Psi\| \\
& + \|p_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) \nabla_1 q_1 q_2 \widehat{w} \Psi\| \\
& \leq C (\|p_2 (W_\beta - U_{0,\beta})(x_1 - x_2)\|_{\text{op}} + \|p_2 \nabla_1 h_{0,\beta}(x_1 - x_2)\|_{\text{op}}) \\
& \leq C \|\varphi\|_\infty (N^{-1+\beta} + N^{-1} (\ln(N))^{1/2}),
\end{aligned}$$

and similarly

$$\begin{aligned}
& \|\nabla_1 q_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) q_1 p_2 \widehat{w}_1 \Psi\| \leq \|q_2 (\Delta_1 h_{0,\beta}(x_1 - x_2)) q_1 p_2 \widehat{w}_1 \Psi\| \\
& + \|q_2 (\nabla_1 h_{0,\beta}(x_1 - x_2)) \nabla_1 q_1 p_2 \widehat{w}_1 \Psi\| \\
& \leq C (\|p_2 (W_\beta - U_{0,\beta})(x_1 - x_2)\|_{\text{op}} + \|\widehat{w}_1\|_{\text{op}} \|p_2 \nabla_1 h_{0,\beta}(x_1 - x_2)\|_{\text{op}}) \\
& \leq C \|\varphi\|_\infty (N^{-1+\beta} + \|\widehat{w}\|_{\text{op}} N^{-1} (\ln(N))^{1/2}).
\end{aligned}$$

Moreover, we estimate

$$\begin{aligned}\|p_2(\nabla_1 h_{0,\beta}(x_1 - x_2))q_1 q_2 \widehat{w}\Psi\| &\leq C\|\varphi\|_\infty \|\nabla_1 h_{0,\beta}\|_2 \leq C\|\varphi\|_\infty N^{-1}(\ln(N))^{1/2} \\ \|q_2(\nabla_1 h_{0,\beta}(x_1 - x_2))q_1 p_2 \widehat{w}\Psi\| &\leq C\|\varphi\|_\infty \|\nabla_1 h_{0,\beta}\|_2 \leq C\|\varphi\|_\infty N^{-1}(\ln(N))^{1/2}.\end{aligned}$$

Hence, we obtain, for any $p > 1$,

$$\begin{aligned}(3.71) + (3.73) &\leq C_p \|\varphi\|_\infty N^{1+\frac{1-2d}{2}\frac{p-1}{p}} \left(N^{-1+\beta} + \|\widehat{w}\|_{\text{op}} N^{-1}(\ln(N))^{1/2} \right)^{\frac{p-1}{p}} \\ &\quad \times \left(N^{-1}(\ln(N))^{1/2} \right)^{1/p}.\end{aligned}$$

For d large enough, the right hand side can be bounded by N^{-1} , that is

$$(3.71) + (3.73) \leq C\|\varphi\|_\infty N^{-1}.$$

For (3.70) we use that $\nabla_2 h_{0,\beta}(x_1 - x_2) = -\nabla_1 h_{0,\beta}(x_1 - x_2)$, Cauchy Schwarz and $ab \leq a^2 + b^2$ and get

$$(3.70) \leq \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 + N^2 \|p_2(\nabla_2 h_{0,\beta}(x_1 - x_2)) \widehat{w} q_1 q_2 \Psi\|^2. \quad (3.74)$$

$\|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2$ can be bounded using Lemma 3.5.10.

Integration by parts and Lemma 2.0.5 (c) as well as $(a+b)^2 \leq 2a^2 + 2b^2$ gives for the second summand

$$\begin{aligned}N^2 \|p_1(\nabla_1 h_{0,\beta}(x_1 - x_2))q_1 q_2 \widehat{w}\Psi\|^2 &\leq 2N^2 \|p_1 h_{0,\beta}(x_1 - x_2) \nabla_1 q_1 q_2 \widehat{w}\Psi\|^2 \\ &\quad + 2N^2 \|\langle \varphi(x_1) \rangle \langle \nabla_1 \varphi(x_1) \rangle h_{0,\beta}(x_1 - x_2) q_1 q_2 \widehat{w}\Psi\|^2 \\ &\leq 2N^2 \|p_1 h_{0,\beta}(x_1 - x_2) q_2 (p_1 \widehat{w}_1 + q_1 \widehat{w}) \mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 \quad (3.75)\end{aligned}$$

$$+ 2N^2 \|p_1 h_{0,\beta}(x_1 - x_2) q_2 p_1 \widehat{w}_1 \mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 \quad (3.76)$$

$$+ 2N^2 \|p_1 h_{0,\beta}(x_1 - x_2) q_2 q_1 \widehat{w} \mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 \quad (3.77)$$

$$+ 2N^2 \|\langle \varphi(x_1) \rangle \langle \nabla_1 \varphi(x_1) \rangle h_{0,\beta}(x_1 - x_2) q_1 q_2 \widehat{w}\Psi\|^2. \quad (3.78)$$

For (3.75) we use Lemma 2.0.7, Lemma 2.0.5 (e) with Lemma 3.5.3 (c) and then Lemma 3.5.10.

$$\begin{aligned}(3.75) &\leq CN^2 \|p_1 h_{0,\beta}(x_1 - x_2)\|_{\text{op}}^2 \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 \\ &\leq \mathcal{K}(\varphi, A.) \left(\langle \Psi, \widehat{n}^\varphi \Psi \rangle + N^{-1/6} \ln(N) \right. \\ &\quad \left. + \inf \left\{ \left| \mathcal{E}_{V_N}(\Psi) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi) \right|, \left| \mathcal{E}_{W_\beta}(\Psi) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi) \right| + N^{-2\beta} \ln(N) \right\} \right).\end{aligned}$$

Let $s_1 \in \{p_1, q_1\}$ and let $\hat{d} \in \{\hat{w}, \hat{w}_1\}$. Note that $\|\hat{d}\|_{\text{op}} = \|\hat{w}\|_{\text{op}}$. Then, (3.76) and (3.77) can be estimated as

$$\begin{aligned}
(3.76), (3.77) &\leq 2N^2 \|\nabla_1 q_1 \Psi\|^2 \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \hat{d} s_1 q_2 h_{0,\beta}(x_1 - x_2) p_1 h_{0,\beta}(x_1 - x_2) q_2 s_1 \hat{d} \mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 \\
&\leq C_p N^{2+2\frac{1-2d}{2}\frac{p-1}{p}} \|\nabla_1 q_1 \Psi\|^2 \|\nabla_1 \hat{d} s_1 q_2 h_{0,\beta}(x_1 - x_2) p_1 h_{0,\beta}(x_1 - x_2) q_2 s_1 \hat{d} \mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^{2\frac{p-1}{p}} \\
&\quad \times \|\hat{d} s_1 q_2 h_{0,\beta}(x_1 - x_2) p_1 h_{0,\beta}(x_1 - x_2) q_2 s_1 \hat{d} \mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^{\frac{2}{p}} \\
&\leq C_p N^{2+2\frac{1-2d}{2}\frac{p-1}{p}} \|\nabla_1 q_1 \Psi\|^2 \|\hat{w}\|_{\text{op}}^2 \|p_1 h_{0,\beta}(x_1 - x_2)\|_{\text{op}}^2 \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 \\
&\quad \times \|\nabla_1 \hat{d} s_1 q_2 h_{0,\beta}(x_1 - x_2) p_1\|_{\text{op}}^{2\frac{p-1}{p}} \|\hat{d} s_1 q_2 h_{0,\beta}(x_1 - x_2) p_1\|_{\text{op}}^{\frac{2}{p}} \\
&\leq \mathcal{K}(\varphi, A.) N^{2\frac{1-2d}{2}\frac{p-1}{p}} \|\hat{w}\|_{\text{op}}^4 \|\nabla_1 s_1 h_{0,\beta}(x_1 - x_2) p_1\|_{\text{op}}^{2\frac{p-1}{p}} \|h_{0,\beta}(x_1 - x_2) p_1\|_{\text{op}}^{\frac{2}{p}} \\
&\leq \mathcal{K}(\varphi, A.) N^{2\frac{1-2d}{2}\frac{p-1}{p}} \|\hat{w}\|_{\text{op}}^4 (\|\nabla \varphi\| \|\nabla_1 h_{0,\beta}\| + \|h_{0,\beta}\|)^{2\frac{p-1}{p}} \|h_{0,\beta}\|_{\text{op}}^{\frac{2}{p}} \\
&\leq \mathcal{K}(\varphi, A.) \|\hat{w}\|_{\text{op}}^4 (\|\nabla \varphi\|^2 + \ln(N))^{\frac{p-1}{p}} N^{2\frac{1-2d}{2}\frac{p-1}{p}-2}.
\end{aligned}$$

Here, we used, for $s_1 \in \{p_1, 1 - p_1\}$,

$$\begin{aligned}
\|\nabla_1 s_1 h_{0,\beta}(x_1 - x_2) p_1\|_{\text{op}} &\leq \|\nabla_1 p_1 h_{0,\beta}(x_1 - x_2) p_1\|_{\text{op}} + \|\nabla_1 h_{0,\beta}(x_1 - x_2) p_1\|_{\text{op}} \\
&\leq \|\varphi\|_{\infty} (\|\nabla \varphi\| \|h_{0,\beta}\| + \|\nabla h_{0,\beta}\|)
\end{aligned}$$

and then applied Lemma 2.0.5 (e).

For d large enough, we obtain

$$(3.76) + (3.77) \leq \mathcal{K}(\varphi, A.) N^{-2}.$$

Line (3.78) can be bounded by

$$\begin{aligned}
(3.78) &\leq N^2 \|h_{0,\beta}(x_1 - x_2) \nabla_1 p_1\|_{\text{op}}^2 \|q_1 q_2 \hat{w} \Psi\|^2 \leq N^2 \|h_{0,\beta}\|^2 \|\nabla \varphi\|_{\infty}^2 \|q_1 \hat{w}\|_{\text{op}}^2 \|q_1 \Psi\|^2 \\
&\leq C \|\nabla \varphi\|_{\infty}^2 \langle\langle \Psi \hat{n} \Psi \rangle\rangle.
\end{aligned}$$

For (3.72) we use Lemma 2.0.10 with $\Omega = \mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi$, $O_{1,2} = N q_2 (\nabla_2 h_{0,\beta}(x_1 - x_2)) p_2$ and $\chi = \hat{w} q_1 \Psi$.

$$(3.72) \leq \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 \quad (3.79)$$

$$+ 2N \|q_2 (\nabla_2 h_{0,\beta}(x_1 - x_2)) \hat{w} q_1 p_2 \Psi\|^2 \quad (3.80)$$

$$+ N^2 |\langle\langle \Psi, q_1 q_3 \hat{w} (\nabla_2 h_{0,\beta}(x_1 - x_2)) p_2 p_3 (\nabla_3 h_{0,\beta}(x_1 - x_3)) \hat{w} q_1 q_2 \Psi \rangle\rangle|. \quad (3.81)$$

Line (3.80) is bounded by

$$\begin{aligned}
(3.80) &\leq C \|\varphi\|_{\infty}^2 N \|(\nabla_2 h_{0,\beta}(x_1 - x_2)) p_2\|_{\text{op}}^2 \|\hat{w} q_1\|_{\text{op}}^2 \\
&\leq C \|\varphi\|_{\infty}^2 N \|\nabla_2 h_{0,\beta}(x_1 - x_2)\|^2 \leq C \|\varphi\|_{\infty}^2 N^{-1} \ln(N).
\end{aligned}$$

(3.79)+(3.81) is bounded by

$$\|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 + N^2 \|p_2(\nabla_2 h_{0,\beta}(x_1 - x_2)) \widehat{w} q_1 q_2 \Psi\|^2.$$

Both terms have been controlled above (see (3.74)). In total, we obtain

$$\begin{aligned} N |\langle\langle \Psi p_1 q_2 Z_\beta^\varphi(x_1, x_2) \widehat{w} q_1 q_2 \Psi \rangle\rangle| &\leq \mathcal{K}(\varphi, A.) \left(\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + N^{-1/6} \ln(N) \right. \\ &\quad \left. + \inf \left\{ \left| \mathcal{E}_{V_N}(\Psi) - \mathcal{E}_{bV_N}^{GP}(\varphi) \right|, \left| \mathcal{E}_{W_\beta}(\Psi) - \mathcal{E}_{bW_\beta}^{GP}(\varphi) \right| + N^{-2\beta} \ln(N) \right\} \right). \end{aligned}$$

□

Using this Lemma, it follows that there exists an $\eta > 0$ such that

$$\gamma_b^<(\Psi_t, \varphi_t) \leq \mathcal{K}(\varphi_t, A_t) \left(\langle\langle \Psi_t, \widehat{n}^{\varphi_t} \Psi_t \rangle\rangle + N^{-\eta} + \left| \mathcal{E}_{W_\beta}(\Psi_0) - \mathcal{E}_{bW_\beta}^{GP}(\varphi_0) \right| \right).$$

This proves Lemma 3.4.6.

3.5.5 Estimates for the functional γ

Lemma 3.5.8 *Let $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C})$, $\|\Psi\| = 1$ and let $\|\nabla_1 \Psi\|$ uniformly bounded in N . Let $V \in L^\infty(\mathbb{R}^2, \mathbb{R})$. Then,*

$$\|p_1 \mathbb{1}_{\text{supp}(V_N)}(x_1 - x_2)\|_{\text{op}} \leq C \|\varphi\|_\infty e^{-N}, \quad (3.82)$$

$$\|V_N(x_1 - x_2)\Psi\| \leq \mathcal{K}(\varphi, A.) e^N \sqrt{N}, \quad (3.83)$$

$$\|p_1 V_N(x_1 - x_2)\Psi\| \leq \mathcal{K}(\varphi, A.) \sqrt{N}. \quad (3.84)$$

Proof: We have

$$\|p_1 \mathbb{1}_{\text{supp}(V_N)}(x_1 - x_2)\|_{\text{op}}^2 \leq \|\varphi\|_\infty^2 \|\mathbb{1}_{\text{supp}(V_N)}\|_1 \leq C \|\varphi\|_\infty^2 e^{-2N}.$$

For the second line, we first estimate

$$\|V_N(x_1 - x_2)\Psi\| \leq C e^{2N} \|\mathbb{1}_{\text{supp}(V_N)}(x_1 - x_2)\Psi\|.$$

We like to recall the two dimensional Sobolev inequality (see [38], Theorem 8.5)

$$\|\rho\|_p^2 \leq C_p (\|\rho\|^2 + \|\nabla \rho\|^2) \quad (3.85)$$

which holds for any $\rho \in H^1(\mathbb{R}^2, \mathbb{C})$ and any $2 \leq p < \infty$. The constant C_p can be estimated as (see [38], Theorem 8.5)

$$C_p \leq \left[p^{1-2/p} (p-1)^{-1+\frac{1}{p}} ((p-2)/8\pi)^{1/2-1/p} \right]^2. \quad (3.86)$$

We will set $p = N$. By the inequality above, we obtain $C_N \leq CN$. We use this inequality in the x_1 variable and obtain together with Hölder's inequality, as in the proof of Lemma 3.5.5,

$$\begin{aligned} & \|\mathbb{1}_{\text{supp}(V_N)}(x_1 - x_2)\Psi\|^2 \\ & \leq \|\mathbb{1}_{\text{supp}(V_N)}\|_{\frac{N}{N-1}} \int d^2x_2 \dots d^2x_N \left(\int d^2x_1 |\Psi(x_1, \dots, x_N)|^{2N} \right)^{1/N} \\ & \leq CN e^{-2N \frac{N-1}{N}} \int d^2x_2 \dots d^2x_N \left(\int d^2x_1 |\nabla_1 \Psi(x_1, \dots, x_N)|^2 + \int d^2x_1 |\Psi(x_1, \dots, x_N)|^2 \right) \\ & \leq CN e^{-2N} (\|\nabla_1 \Psi\|^2 + \|\Psi\|^2). \end{aligned}$$

For the last inequality, we estimate

$$\begin{aligned} \|p_1 V_N(x_1 - x_2)\Psi\| &= \|p_1 \mathbb{1}_{\text{supp}(V_N)}(x_1 - x_2) V_N(x_1 - x_2)\Psi\| \\ &\leq C e^{2N} \|p_1 \mathbb{1}_{\text{supp}(V_N)}(x_1 - x_2)\|_{\text{op}} \|\mathbb{1}_{\text{supp}(V_N)}(x_1 - x_2)\Psi\|. \end{aligned}$$

Combining all estimates then yields the Lemma. □

Remark 3.5.9 For V nonnegative, we were able to derive the improved bound $\|p_1 V_N(x_1 - x_2)\Psi\| \leq \mathcal{K}(\varphi, A.) N^{-1/2}$, see Lemma 7.8. in [25].

Control of γ_b Recall that

$$\begin{aligned} \gamma_b(\Psi, \varphi) &= -N(N-1) \Im \left(\langle\langle \Psi, \tilde{Z}_\beta^\varphi(x_1, x_2) \hat{r} \Psi \rangle\rangle \right) \\ &\quad - N(N-1) \Im \left(\langle\langle \Psi, g_\beta(x_1 - x_2) \hat{r} \mathcal{Z}^\varphi(x_1, x_2) \Psi \rangle\rangle \right). \end{aligned}$$

Estimate (3.82) yields to the bound $\|p_1 \mathcal{Z}^\varphi(x_1, x_2)\Psi\| \leq \mathcal{K}(\varphi, A.) N^{1/2}$. Therefore, the second line of γ_b is controlled by

$$\begin{aligned} & N^2 \|g_\beta(x_1 - x_2) p_1\|_{\text{op}} \|\hat{r}\|_{\text{op}} \|p_1 \mathcal{Z}^\varphi(x_1, x_2)\Psi\| \\ & \leq \mathcal{K}(\varphi, A.) N^{5/2} \|g_\beta\| \|\hat{r}\|_{\text{op}} \leq \mathcal{K}(\varphi, A.) N^{3/2+\xi-\beta}. \end{aligned}$$

The first line of γ_b can be bounded with (3.37) and $f_\beta = 1 - g_\beta$ by

$$\begin{aligned} & N(N-1) \left| \Im \left(\langle\langle \Psi, \tilde{Z}_\beta^\varphi(x_1, x_2) \hat{r} \Psi \rangle\rangle \right) \right| \\ & \leq N^2 \left| \Im \left(\langle\langle \Psi, \left(M_\beta(x_1 - x_2) f_\beta(x_1 - x_2) - \frac{N}{N-1} (\|M_\beta f_\beta\|_1 |\varphi(x_1)|^2 + \|M_\beta f_\beta\|_1 |\varphi(x_2)|^2) \right) \hat{r} \Psi \rangle\rangle \right) \right| \end{aligned} \tag{3.87}$$

$$+ \frac{N^2}{N-1} \left| \langle\langle \Psi, (\|NM_\beta f_\beta\|_1 - b_{V_N}) (|\varphi(x_1)|^2 + |\varphi(x_2)|^2) \hat{r} \Psi \rangle\rangle \right| \tag{3.88}$$

$$+ \frac{N^2}{N-1} \left| \langle\langle \Psi, (b_{V_N} |\varphi(x_1)|^2 + b_{V_N} |\varphi(x_2)|^2) g_\beta(x_1 - x_2) \hat{r} \Psi \rangle\rangle \right|. \tag{3.89}$$

Since $M_\beta f_\beta \in \mathcal{V}_\beta$, (3.87) is of the same form as $\gamma_b^<(\Psi, \varphi)$. Using Lemma 3.3.6 (h), the second term is controlled by

$$(3.88) \leq C\|\varphi\|_\infty^2 N (N\|M_\beta f_\beta\|_1 - b_{V_N}) \|\hat{r}\|_{\text{op}} \leq C\|\varphi\|_\infty^2 N^{-1+\xi} \ln(N).$$

The last term is controlled by

$$(3.89) \leq CN\|\varphi\|_\infty^2 \|g_\beta(x_1 - x_2)p_1\|_{\text{op}} \|\hat{r}\|_{\text{op}} \leq C\|\varphi\|_\infty^3 N^{\xi-\beta}.$$

Choosing β sufficiently big, we obtain

$$|\gamma_b(\Psi, \varphi)| \leq \mathcal{K}(\varphi, A.) \left(\langle\langle \Psi, \hat{m}\Psi \rangle\rangle + |\mathcal{E}_{V_N}(\Psi) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi)| + N^{-\eta} \right)$$

for some $\eta > 0$.

Control of γ_c Recall that

$$\gamma_c(\Psi, \varphi) = -4N(N-1) \langle\langle \Psi, (\nabla_1 g_\beta(x_1 - x_2)) \nabla_1 \hat{r}\Psi \rangle\rangle.$$

Using $\hat{r} = (p_2 + q_2)\hat{r} = p_2\hat{r} + p_1q_2\hat{m}^a$ and $\nabla_1 g_\beta(x_1 - x_2) = -\nabla_2 g_\beta(x_1 - x_2)$, integration by parts yields to

$$|\gamma_c(\Psi, \varphi)| \leq 4N^2 |\langle\langle \Psi, g_\beta(x_1 - x_2) \nabla_1 \nabla_2 (p_2\hat{r} + p_1q_2\hat{m}^a) \Psi \rangle\rangle| \quad (3.90)$$

$$+ 4N^2 |\langle\langle \nabla_2 \Psi, g_\beta(x_1 - x_2) \nabla_1 p_2 \hat{r} \Psi \rangle\rangle| \quad (3.91)$$

$$+ 4N^2 |\langle\langle \nabla_2 \Psi, g_\beta(x_1 - x_2) \nabla_1 p_1 q_2 \hat{m}^a \Psi \rangle\rangle|. \quad (3.92)$$

We begin with

$$(3.90) \leq CN^2 \|g_\beta\| \|\nabla \varphi\|_\infty (\|\nabla_1 \hat{r}\varphi\| + \|\nabla_2 q_2 \hat{m}^a \Psi\|) \\ \leq CN^{2-\beta} \|\nabla \varphi\|_\infty (\|\nabla_1 \hat{r}\varphi\| + \|\nabla_2 q_2 \hat{m}^a \Psi\|).$$

Let $s_1, t_1 \in \{p_1, q_1\}$, $s_2, t_2 \in \{p_2, q_2\}$. Inserting the identity $1 = (p_1 + q_1)(p_2 + q_2)$, we obtain, for $a \in \{-2, -1, 0, 1, 2\}$,

$$\|\nabla_1 \hat{r}\Psi\| \leq C \sup_{s_1, s_2, t_1, t_2, a} \|\hat{r}_a s_1 s_2 \nabla_1 t_1 t_2 \Psi\| \leq C \sup_{t_1, a} \|\hat{r}_a\|_{\text{op}} \|\nabla_1 t_1 \Psi\| \\ \leq CN^{-1+\xi}.$$

In analogy $\|\nabla_2 q_2 \hat{m}^a \Psi\| \leq C\|\hat{m}^a\|_{\text{op}} \leq CN^{-1+\xi}$. This yields the bound

$$(3.90) \leq \mathcal{K}(\varphi, A.) N^{1-\beta+\xi}.$$

Furthermore, (3.91) is bounded by

$$(3.91) \leq 4N^2 \|\nabla_2 \Psi\| \|g_\beta\| \|\nabla \varphi\|_\infty \|\nabla_1 \hat{r}\Psi\| \leq C\|\nabla \varphi\|_\infty N^{1+\xi-\beta}. \quad (3.93)$$

Similarly, we obtain

$$(3.92) \leq 4N^2 \|\nabla_2 \Psi\| \|g_\beta\| \|\nabla \varphi\|_\infty \|q_2 \hat{m}^a \Psi\| \leq C\|\nabla \varphi\|_\infty N^{1+\xi-\beta}.$$

It follows that $|\gamma_c(\Psi, \varphi)| \leq \mathcal{K}(\varphi, A.) N^{1+\xi-\beta}$.

Control of γ_d To control γ_d and γ_e we will use the notation

$$\begin{aligned} m^c(k) &= m^a(k) - m^a(k+1) & m^d(k) &= m^a(k) - m^a(k+2) \\ m^e(k) &= m^b(k) - m^b(k+1) & m^f(k) &= m^b(k) - m^b(k+2). \end{aligned} \quad (3.94)$$

Since the second k -derivative of m is given by (see (3.52) for the first derivative)

$$m(k)'' = \begin{cases} -1/(4\sqrt{k^3 N}), & \text{for } k \geq N^{1-2\xi}; \\ 0, & \text{else.} \end{cases}$$

It is easy to verify that

$$\|\widehat{m}_j^x\|_{\text{op}} \leq CN^{-2+3\xi} \text{ for } x \in \{c, d, e, f\}. \quad (3.95)$$

Recall that

$$\begin{aligned} \gamma_d(\Psi, \varphi) &= 2N(N-1)(N-2)\Im(\langle\langle \Psi, g_\beta(x_1 - x_2) [V_N(x_1 - x_3), \widehat{r}] \Psi \rangle\rangle) \\ &\quad + N(N-1)(N-2)\Im(\langle\langle \Psi, g_\beta(x_1 - x_2) [b_{V_N}|\varphi|^2(x_3), \widehat{r}] \Psi \rangle\rangle). \end{aligned}$$

Since $p_j + q_j = 1$, we can rewrite \widehat{r} as

$$\widehat{r} = \widehat{m}^b p_1 p_2 + \widehat{m}^a (p_1 q_2 + q_1 p_2) = (\widehat{m}^b - 2\widehat{m}^a) p_1 p_2 + \widehat{m}^a (p_1 + p_2).$$

Thus,

$$\begin{aligned} |\gamma_d(\Psi, \varphi)| &\leq CN^3 |\langle\langle \Psi, g_\beta(x_1 - x_2) [V_N(x_1 - x_3), (\widehat{m}^b - 2\widehat{m}^a)p_1 p_2 + \widehat{m}^a(p_1 + p_2)] \Psi \rangle\rangle| \\ &\quad + CN^3 |\langle\langle \Psi, g_\beta(x_1 - x_2) [b_{V_N}|\varphi|^2(x_3), \widehat{r}] \Psi \rangle\rangle| \\ &\leq CN^3 |\langle\langle \Psi, g_\beta(x_1 - x_2) p_2 [V_N(x_1 - x_3), \widehat{m}^a] \Psi \rangle\rangle| \end{aligned} \quad (3.96)$$

$$+ CN^3 |\langle\langle \Psi, g_\beta(x_1 - x_2) V_N(x_1 - x_3) (\widehat{m}^b - 2\widehat{m}^a) p_1 p_2 \Psi \rangle\rangle| \quad (3.97)$$

$$+ CN^3 |\langle\langle \Psi, g_\beta(x_1 - x_2) (\widehat{m}^b - 2\widehat{m}^a) p_1 p_2 V_N(x_1 - x_3) \Psi \rangle\rangle| \quad (3.98)$$

$$+ CN^3 |\langle\langle \Psi, g_\beta(x_1 - x_2) \widehat{m}^a p_1 V_N(x_1 - x_3) \Psi \rangle\rangle| \quad (3.99)$$

$$+ CN^3 |\langle\langle \Psi, g_\beta(x_1 - x_2) V_N(x_1 - x_3) \widehat{m}^a p_1 \Psi \rangle\rangle| \quad (3.100)$$

$$+ CN^3 |\langle\langle \Psi, g_\beta(x_1 - x_2) [b_{V_N}|\varphi|^2(x_3), \widehat{r}] \Psi \rangle\rangle|. \quad (3.101)$$

Using Lemma 2.0.5 (d), we obtain the following estimate:

$$\begin{aligned} (3.96) &= CN^3 |\langle\langle \Psi, g_\beta(x_1 - x_2) p_2 [V_N(x_1 - x_3), p_1 p_3 \widehat{m}^d + p_1 q_3 \widehat{m}^c + q_1 p_3 \widehat{m}^c] \Psi \rangle\rangle| \\ &\leq CN^3 |\langle\langle \Psi, V_N(x_1 - x_3) g_\beta(x_1 - x_2) p_2 \mathbb{1}_{\text{supp}(V_N)}(x_1 - x_3) \\ &\quad \times (p_1 p_3 \widehat{m}^d + p_1 q_3 \widehat{m}^c + q_1 p_3 \widehat{m}^c) \Psi \rangle\rangle| \\ &\quad + CN^3 |\langle\langle \Psi, g_\beta(x_1 - x_2) p_2 (p_1 p_3 \widehat{m}^d + p_1 q_3 \widehat{m}^c + q_1 p_3 \widehat{m}^c) V_N(x_1 - x_3) \Psi \rangle\rangle|. \end{aligned}$$

Both lines are bounded by

$$\begin{aligned} &CN^3 \|V_N(x_1 - x_3) \Psi\| \|g_\beta(x_1 - x_2) p_2\|_{\text{op}} \\ &(2\|\mathbb{1}_{\text{supp}(V_N)}(x_1 - x_3) p_1\|_{\text{op}} + \|\mathbb{1}_{\text{supp}(V_N)}(x_1 - x_3) p_3\|_{\text{op}}) (\|\widehat{m}^d\|_{\text{op}} + \|\widehat{m}^c\|_{\text{op}}). \end{aligned}$$

In view of Lemma 2.0.5 (e) with Lemma 3.3.6 (i), $\|g_\beta(x_1 - x_2)p_2\|_{\text{op}} \leq \|\varphi\|_\infty \|g_\beta\| \leq C\|\varphi\|_\infty N^{-\beta}$. Using (3.95), together with

$$\|\mathbf{1}_{\text{supp}(V_N)}(x_1 - x_3)p_1\|_{\text{op}} \|V_N(x_1 - x_3)\Psi\| \leq N^{1/2} \mathcal{K}(\varphi, A.),$$

we obtain

$$(3.96) \leq \mathcal{K}(\varphi, A.) N^{3/2+3\xi-\beta}.$$

We continue with

$$\begin{aligned} & (3.97) + (3.98) + (3.99) \\ & \leq CN^3 \|V_N(x_1 - x_3)\Psi\| \|g_\beta(x_1 - x_2)p_2\|_{\text{op}} \|\mathbf{1}_{\text{supp}(V_N)}(x_1 - x_3)p_1\|_{\text{op}} \|(\widehat{m}^b - 2\widehat{m}^a)\|_{\text{op}} \\ & + CN^3 \|g_\beta(x_1 - x_2)p_2\|_{\text{op}} \|\widehat{m}^b - 2\widehat{m}^a\|_{\text{op}} \|p_1 V_N(x_1 - x_3)\Psi\| \\ & + CN^3 \|g_\beta(x_1 - x_2)p_1\|_{\text{op}} \|\widehat{m}^a\|_{\text{op}} \|p_1 V_N(x_1 - x_3)\Psi\| \\ & \leq \mathcal{K}(\varphi, A.) N^{5/2+\xi-\beta}. \end{aligned}$$

Next, we estimate (3.100). The support of the function $g_\beta(x_1 - x_2)V_N(x_1 - x_3)$ is such that $|x_1 - x_2| \leq CN^{-\beta}$, as well as $|x_1 - x_3| \leq Ce^{-N}$. Therefore, $g_\beta(x_1 - x_2)V_N(x_1 - x_3) \neq 0$ implies $|x_2 - x_3| \leq CN^{-\beta}$. We estimate

$$\begin{aligned} (3.100) & = CN^3 \left| \langle \Psi, g_\beta(x_1 - x_2)V_N(x_1 - x_3)p_1 \mathbf{1}_{B_{CN^{-\beta}}(0)}(x_2 - x_3)\widehat{m}^a \Psi \rangle \right| \\ & \leq CN^3 \|p_1 V_N(x_1 - x_3)g_\beta(x_1 - x_2)\Psi\| \|\mathbf{1}_{B_{CN^{-\beta}}(0)}(x_2 - x_3)\widehat{m}^a \Psi\| \\ & \leq CN^3 \|p_1 \mathbf{1}_{\text{supp}(V_N)}(x_1 - x_3)\|_{\text{op}} \|g_\beta(x_1 - x_2)V_N(x_1 - x_3)\Psi\| \|\mathbf{1}_{B_{CN^{-\beta}}(0)}(x_2 - x_3)\widehat{m}^a \Psi\| \\ & \leq CN^{7/2} \|g_\beta\|_\infty \|\mathbf{1}_{B_{CN^{-\beta}}(0)}\|_{\frac{2}{p-1}}^{\frac{1}{2}} \|\nabla_1 \widehat{m}^a \Psi\|_{\frac{p-1}{p}} \|\widehat{m}^a \Psi\|_{\frac{1}{p}} \\ & \leq C_p N^{7/2} \|g_\beta\|_\infty N^{-\beta/2} \|\nabla_1 \widehat{m}^a \Psi\|^{1/2} \|\widehat{m}^a \Psi\|^{1/2} \\ & \leq \mathcal{K}(\varphi, A.) N^{5/2+\xi-\beta/2}. \end{aligned}$$

In the fourth line, we applied Sobolev inequality as in the proof of Lemma 3.5.5, then setting $p = 2$. Furthermore, we used $\|\nabla_1 \widehat{m}^a \Psi\|^{1/2} \|\widehat{m}^a \Psi\|^{1/2} \leq \mathcal{K}(\varphi, A.) N^{-1+\xi}$, as well as $\|g_\beta\|_\infty \leq C$, see Lemma 3.3.6.

Using Lemma 2.0.5 (d), (3.101) can be bounded by

$$\begin{aligned} & CN^3 \left| \langle \Psi, g_\beta(x_1 - x_2) [b_{V_N}|\varphi|^2(x_3), p_1 p_2 (\widehat{r} - \widehat{r}_2) + (p_1 q_2 + q_1 p_2)(\widehat{r} - \widehat{r}_1)] \Psi \rangle \right| \\ & \leq CN^3 \|\varphi\|_\infty^2 (\|\widehat{r} - \widehat{r}_2\|_{\text{op}} + \|\widehat{r} - \widehat{r}_1\|_{\text{op}}) \|g_\beta(x_1 - x_2)p_2\|_{\text{op}}. \end{aligned}$$

Note that $\|\widehat{r} - \widehat{r}_2\|_{\text{op}} + \|\widehat{r} - \widehat{r}_1\|_{\text{op}} \leq \sum_{j \in \{c, d, e, f\}} \|\widehat{m}^j\|_{\text{op}} \leq CN^{-2+3\xi}$ holds. With $\|g_\beta(x_1 - x_2)p_2\|_{\text{op}} \leq CN^{-\beta}$, it then follows that

$$|(3.101)| \leq C\|\varphi\|_\infty^2 N^{1+3\xi-\beta}.$$

In total, we obtain, using $\xi < 1/2$,

$$|\gamma_d(\Psi, \varphi)| \leq \mathcal{K}(\varphi, A.) N^{3-\beta/2}.$$

Control of γ_e Recall that

$$\begin{aligned}\gamma_e(\Psi, \varphi) &= -\frac{1}{2}N(N-1)(N-2)(N-3) \\ &\quad \Im(\langle\langle \Psi, g_\beta(x_1 - x_2) [V_N(x_3 - x_4), \hat{r}] \Psi \rangle\rangle).\end{aligned}$$

Using symmetry, Lemma 2.0.5 (d) and Notation (3.94), γ_e is bounded by

$$\begin{aligned}\gamma_e(\Psi, \varphi) &\leq N^4 |\langle\langle \Psi, g_\beta(x_1 - x_2) [V_N(x_3 - x_4), \hat{m}^c p_1 p_2 p_3 p_4 + 2\hat{m}^d p_1 p_2 p_3 p_4 \\ &\quad + 2\hat{m}^e p_1 q_2 p_3 p_4 + 4\hat{m}^f p_1 q_2 p_3 q_4] \Psi \rangle\rangle| \\ &\leq 4N^4 \|V_N(x_3 - x_4)\Psi\| \|\mathbf{1}_{\text{supp}(V_N)}(x_3 - x_4)p_3\|_{\text{op}} \|g_\beta(x_1 - x_2)p_1\|_{\text{op}} \\ &\quad \times (\|\hat{m}^c\|_{\text{op}} + \|\hat{m}^d\|_{\text{op}} + \|\hat{m}^e\|_{\text{op}} + \|\hat{m}^f\|_{\text{op}}).\end{aligned}$$

We get with (3.95), Lemma 3.3.6 and Lemma 2.0.5 that

$$|\gamma_e(\Psi, \varphi)| \leq \mathcal{K}(\varphi, A.) N^{5/2+3\xi-\beta}.$$

Control of γ_f Recall that

$$\gamma_f(\Psi, \varphi) = 2N(N-1) \frac{N-2}{N-1} \Im(\langle\langle \Psi, g_\beta(x_1 - x_2) [b_{V_N}|\varphi|^2(x_1), \hat{r}] \Psi \rangle\rangle).$$

We obtain the estimate

$$|\gamma_f(\Psi, \varphi)| \leq \mathcal{K}(\varphi, A.) N^2 \|g_\beta\| \|\hat{r}\|_{\text{op}} \leq \mathcal{K}(\varphi, A.) N^{1+\xi-\beta}. \quad (3.102)$$

Summary of the estimates Collecting all estimates, we get with $\xi < 1/2$

$$|\gamma_c(\Psi, \varphi)| + |\gamma_d(\Psi, \varphi)| + |\gamma_e(\Psi, \varphi)| + |\gamma_f(\Psi, \varphi)| \leq \mathcal{K}(\varphi, A.) \left(N^{4-\beta} + N^{3-\frac{\beta}{2}} \right). \quad (3.103)$$

Choosing β sufficiently large, we obtain the desired decay and hence Lemma 3.4.10.

3.5.6 Energy estimates

Lemma 3.5.10 *Let $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap H^1(\mathbb{R}^{2N}, \mathbb{C})$, $\|\Psi\| = 1$ with $\|\nabla_1 \Psi\| \leq \mathcal{K}(\varphi, A.)$. Let $\varphi \in H^3(\mathbb{R}^2, \mathbb{C})$, $\|\varphi\| = 1$. Let $W_\beta \in \mathcal{V}_\beta$ as in Definition 3.3.4 and let V satisfy Assumption 3.2.3. Assume $-(1-\epsilon)\Delta + \frac{1}{2}W \geq 0$ on $L^2(\mathbb{R}^2, \mathbb{C})$ for some $\epsilon > 0$. Let the sets $\mathcal{A}_1^{(d)}, \bar{\mathcal{B}}_1^{(d)}$ be defined as in Definition 3.5.4. Then, for d large enough,*

$$\begin{aligned}\|\mathbf{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 &\leq \mathcal{K}(\varphi, A.) \left(\langle\langle \Psi, \hat{n}^\varphi \Psi \rangle\rangle + N^{-1/6} \ln(N) \right. \\ &\quad \left. + \inf \left\{ \left| \mathcal{E}_{V_N}(\Psi) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi) \right|, \left| \mathcal{E}_{W_\beta}(\Psi) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi) \right| + N^{-2\beta} \ln(N) \right\} \right).\end{aligned}$$

Proof: We expanding $\mathcal{E}_{W_\beta}(\Psi) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi)$. This yields

$$\begin{aligned}\mathcal{E}_{W_\beta}(\Psi) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi) &= \|\nabla_1 \Psi\|^2 + \frac{N-1}{2} \langle \langle \Psi, W_\beta(x_1 - x_2) \Psi \rangle \rangle \\ &\quad - \|\nabla \varphi\|^2 - \frac{1}{2} b_{W_\beta} \|\varphi^2\|^2 + \langle \langle \Psi, A_t(x_1) \Psi \rangle \rangle - \langle \varphi, A_t \varphi \rangle \\ &= \epsilon \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 + \epsilon \|\mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 + M(\Psi, \varphi) + Q_\beta(\Psi, \varphi),\end{aligned}$$

where we have defined

$$M(\Psi, \varphi) = 2\Re \left(\langle \langle \nabla_1 q_1 \Psi, \mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 p_1 \Psi \rangle \rangle \right) \quad (3.104)$$

$$+ \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 p_1 \Psi\|^2 - \|\nabla \varphi\|^2 \quad (3.105)$$

$$+ \langle \langle \Psi, A_t(x_1) \Psi \rangle \rangle - \langle \varphi, A_t \varphi \rangle, \quad (3.106)$$

$$Q_\beta(\Psi, \varphi) = (1 - \epsilon) \|\mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 + (1 - \epsilon) \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 \quad (3.107)$$

$$+ \frac{N-1}{2} \langle \langle \Psi, (1 - p_1 p_2) W_\beta(x_1 - x_2) (1 - p_1 p_2) \Psi \rangle \rangle \quad (3.108)$$

$$+ \frac{N-1}{2} \langle \langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) p_1 p_2 \Psi \rangle \rangle - \frac{1}{2} N \int_{\mathbb{R}^2} W_\beta(x) d^2 x \|\varphi^2\|^2$$

$$+ (N-1) \Re \langle \langle \Psi, (1 - p_1 p_2) W_\beta(x_1 - x_2) p_1 p_2 \Psi \rangle \rangle.$$

We first consider the first two contributions (3.107) + (3.108). Note that $(1 - p_1 p_2) \Delta_1 (1 - p_1 p_2) = p_1 \Delta_1 p_1 q_2 + p_1 \Delta_1 q_1 q_2 + q_1 q_2 \Delta_1 p_1 + q_1 \Delta_1 q_1$. We hence obtain

$$\begin{aligned}(3.107) &= - (1 - \epsilon) \langle \langle \Psi, q_1 \Delta_1 q_1 \Psi \rangle \rangle + \|\mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 p_1 \Psi\|^2 + 2\Re \left(\langle \langle \nabla_1 p_1 \Psi, \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 q_1 \Psi \rangle \rangle \right) \\ &= - (1 - \epsilon) \langle \langle \Psi, (1 - p_1 p_2) \Delta_1 (1 - p_1 p_2) \Psi \rangle \rangle \\ &\quad + (1 - \epsilon) (\langle \langle \Psi, p_1 \Delta_1 p_1 q_2 \Psi \rangle \rangle + 2\Re (\langle \langle \Psi, q_1 q_2 \Delta_1 p_1 \Psi \rangle \rangle)) \\ &\quad + \|\mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 p_1 \Psi\|^2 + 2\Re \left(\langle \langle \nabla_1 p_1 \Psi, \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 q_1 \Psi \rangle \rangle \right)\end{aligned}$$

Rearranging terms, we obtain

$$(3.107) + (3.108) = \langle \langle \Psi, (1 - p_1 p_2) \left(- (1 - \epsilon) \Delta_1 + \frac{N-1}{2} W_\beta(x_1 - x_2) \right) (1 - p_1 p_2) \Psi \rangle \rangle \quad (3.109)$$

$$+ (1 - \epsilon) (\langle \langle \Psi, p_1 \Delta_1 p_1 q_2 \Psi \rangle \rangle + \langle \langle \Psi, p_1 \Delta_1 q_1 q_2 \Psi \rangle \rangle + \langle \langle \Psi, q_1 q_2 \Delta_1 p_1 \Psi \rangle \rangle) \quad (3.110)$$

$$+ \|\mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 p_1 \Psi\|^2 + 2\Re \left(\langle \langle \nabla_1 p_1 \Psi, \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 q_1 \Psi \rangle \rangle \right). \quad (3.111)$$

Note that the operator inequality $-(1 - \epsilon) \Delta + \frac{1}{2} W \geq 0$ implies by rescaling that (3.109) is nonnegative. Furthermore, it follows

$$|(3.110)| \leq \mathcal{K}(\varphi, A) \langle \langle \Psi, q_1 \Psi \rangle \rangle,$$

and, applying Lemma 3.5.5, part (a),

$$|(3.111)| \leq \mathcal{K}(\varphi, A.) (\|\nabla_1 q_1 \Psi\| + 1) N^{1/2-d}.$$

Define

$$S_\beta(\Psi, \varphi) = (N-1) |\langle\langle \Psi, (1-p_1 p_2) W_\beta(x_1 - x_2) p_1 p_2 \Psi \rangle\rangle| \quad (3.112)$$

$$+ \left| \frac{N-1}{2} \langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) p_1 p_2 \Psi \rangle\rangle - \frac{1}{2} b_{W_\beta} \|\varphi^2\|^2 \right|. \quad (3.113)$$

Applying the estimates above, together with the assumptions $\|\nabla_1 \Psi\| \leq C$, $\|\nabla \varphi\| \leq C$, we can then conclude the bound

$$\begin{aligned} \epsilon \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 \leq & |M(\Psi, \varphi)| + |S_\beta(\Psi, \varphi)| + \left| \mathcal{E}_{W_\beta}(\Psi) - \mathcal{E}_{b_{W_\beta}}^{GP}(\varphi) \right| \\ & + \mathcal{K}(\varphi, A.) (\langle\langle \Psi, q_1 \Psi \rangle\rangle + N^{1/2-d}). \end{aligned}$$

Next, we split up the energy difference $\mathcal{E}_{V_N}(\Psi) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi)$,

$$\begin{aligned} \mathcal{E}_{V_N}(\Psi) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi) = & \|\nabla_1 \Psi\|^2 + \frac{N-1}{2} \langle\langle \Psi, V_N(x_1 - x_2) \Psi \rangle\rangle - \|\nabla \varphi\|^2 \\ & - \frac{b_{V_N}}{2} \|\varphi^2\|^2 + \langle\langle \Psi, A.(x_1) \Psi \rangle\rangle - \langle \varphi, A.\varphi \rangle. \end{aligned}$$

In order to better estimate the terms corresponding to the two-particle interactions, we introduce, for $\mu > d$, the potential $M_\mu(x)$, defined in Definition 3.3.5, and continue with

$$\begin{aligned} \mathcal{E}_{V_N}(\Psi) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi) = & \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 \Psi\|^2 + \|\mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} \mathbb{1}_{\bar{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 + \|\mathbb{1}_{\mathcal{B}_1^{(d)}} \mathbb{1}_{\bar{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 \\ & + \frac{N-1}{2} \langle\langle \Psi, \mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} V_N(x_1 - x_2) \Psi \rangle\rangle \\ & + \frac{1}{2} \langle\langle \Psi, \sum_{j=2}^N \mathbb{1}_{\mathcal{B}_1^{(d)}} (V_N - M_\mu)(x_1 - x_j) \Psi \rangle\rangle \\ & + \frac{1}{2} \langle\langle \Psi, \sum_{j=2}^N \mathbb{1}_{\mathcal{B}_1^{(d)}} M_\mu(x_1 - x_j) \Psi \rangle\rangle - \|\nabla \varphi\|^2 - \frac{b_{V_N}}{2} \|\varphi^2\|^2 \\ & + \langle\langle \Psi, A.(x_1) \Psi \rangle\rangle - \langle \varphi, A.\varphi \rangle. \end{aligned}$$

Using that $q_1 = 1 - p_1$ and symmetry, we obtain for $0 < \epsilon < 1$,

$$\begin{aligned}
& \mathcal{E}_{V_N}(\Psi) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi) \\
&= \epsilon \left(\|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 + \|\mathbb{1}_{\overline{\mathcal{B}}_1^{(d)}} \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 \right) \\
&+ (1 - \epsilon) \left(\|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 + \|\mathbb{1}_{\overline{\mathcal{B}}_1^{(d)}} \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 \right) \\
&+ \frac{N-1}{2} \langle\langle \Psi, \mathbb{1}_{\overline{\mathcal{B}}_1^{(d)}} V_N(x_1 - x_2) \Psi \rangle\rangle \\
&+ \frac{N-1}{2} \langle\langle \Psi, \mathbb{1}_{\mathcal{B}_1^{(d)}} (1 - p_1 p_2) M_\mu(x_1 - x_2) (1 - p_1 p_2) \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \\
&+ \|\mathbb{1}_{\mathcal{B}_1^{(d)}} \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 + \frac{1}{2} \langle\langle \Psi, \sum_{j=2}^N \mathbb{1}_{\mathcal{B}_1^{(d)}} (V_N - M_\mu)(x_1 - x_j) \Psi \rangle\rangle \\
&+ \frac{N-1}{2} \langle\langle \Psi, \mathbb{1}_{\mathcal{B}_1^{(d)}} p_1 p_2 M_\mu(x_1 - x_2) p_1 p_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle - \frac{b_{V_N}}{2} \|\varphi^2\|^2 \\
&+ 2\Re \left(\langle\langle \nabla_1 q_1 \Psi, \mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 p_1 \Psi \rangle\rangle \right) \\
&+ (N-1)\Re \langle\langle \Psi, \mathbb{1}_{\mathcal{B}_1^{(d)}} (1 - p_1 p_2) M_\mu(x_1 - x_2) p_1 p_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \\
&+ \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 p_1 \Psi\|^2 - \|\nabla \varphi\|^2 \\
&+ \langle\langle \Psi, A.(x_1) \Psi \rangle\rangle - \langle \varphi, A.\varphi \rangle \\
&= \epsilon \left(\|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 + \|\mathbb{1}_{\overline{\mathcal{B}}_1^{(d)}} \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 \right) + M(\Psi, \varphi) + \tilde{Q}_\mu(\Psi, \varphi).
\end{aligned}$$

with

$$\begin{aligned}
\tilde{Q}_\mu(\Psi, \varphi) &= \frac{N-1}{2} \langle\langle \Psi, \mathbb{1}_{\mathcal{B}_1^{(d)}} (1 - p_1 p_2) M_\mu(x_1 - x_2) (1 - p_1 p_2) \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \\
&+ (1 - \epsilon) \left(\|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 + \|\mathbb{1}_{\overline{\mathcal{B}}_1^{(d)}} \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 \right) + \frac{N-1}{2} \langle\langle \Psi, \mathbb{1}_{\overline{\mathcal{B}}_1^{(d)}} V_N(x_1 - x_2) \Psi \rangle\rangle \\
&\quad (3.114)
\end{aligned}$$

$$\begin{aligned}
&+ \|\mathbb{1}_{\mathcal{B}_1^{(d)}} \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 + \frac{1}{2} \langle\langle \Psi, \sum_{j=2}^N \mathbb{1}_{\mathcal{B}_1^{(d)}} (V_N - M_\mu)(x_1 - x_j) \Psi \rangle\rangle \\
&+ (N-1)\Re \langle\langle \Psi, \mathbb{1}_{\mathcal{B}_1^{(d)}} (1 - p_1 p_2) M_\mu(x_1 - x_2) p_1 p_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \\
&+ \frac{N-1}{2} \langle\langle \Psi, \mathbb{1}_{\mathcal{B}_1^{(d)}} p_1 p_2 M_\mu(x_1 - x_2) p_1 p_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle - \frac{b_{V_N}}{2} \|\varphi^2\|^2.
\end{aligned} \quad (3.115)$$

The first term in $\tilde{Q}_\mu(\Psi, \varphi)$ is nonnegative. For $\mu > d$ Lemma 3.5.11 below shows that

(3.115) is also nonnegative. Furthermore, we are able to bound, for $0 < \epsilon < 1$,

$$(3.114) = (1 - \epsilon) \left(\|\mathbb{1}_{\mathcal{A}_1^{(d)}} \mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} \nabla_1 \Psi\|^2 + \|\mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} \mathbb{1}_{\bar{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 \right) + \frac{N-1}{2} \langle\langle \Psi, \mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} V_N(x_1 - x_2) \Psi \rangle\rangle \\ - (1 - \epsilon) 2\Re \left(\langle\langle \nabla_1 \Psi, \mathbb{1}_{\mathcal{A}_1^{(d)}} \mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} \nabla_1 p_1 \Psi \rangle\rangle \right) \\ + (1 - \epsilon) \left(\|\mathbb{1}_{\mathcal{A}_1^{(d)}} \mathbb{1}_{\mathcal{B}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 + \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} \nabla_1 p_1 \Psi\|^2 \right)$$

The third line is positive. In analogy to the proof of Lemma 3.5.5, we obtain

$$\|\mathbb{1}_{\mathcal{A}_1^{(d)}} \mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} \nabla_1 p_1 \Psi\| \leq \|\mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} \nabla_1 p_1 \Psi\| \leq \mathcal{K}(\varphi, A.) N^{1-d+\delta}$$

for any $\delta > 0$. This implies

$$2\Re \left(\langle\langle \nabla_1 \Psi, \mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} \mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 p_1 \Psi \rangle\rangle \right) \leq \mathcal{K}(\varphi, A.) N^{1-d+\delta}.$$

Focusing on the first term, we obtain with Corollary 4.3.15

$$(1 - \epsilon) \left(\|\mathbb{1}_{\mathcal{A}_1^{(d)}} \mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} \nabla_1 \Psi\|^2 + \|\mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} \mathbb{1}_{\bar{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 \right) + \frac{N-1}{2} \langle\langle \Psi, \mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} V_N(x_1 - x_2) \Psi \rangle\rangle \\ (3.116)$$

$$= \frac{1}{N} \langle\langle \Psi, \left(-(1 - \epsilon) \sum_{k=1}^N \Delta_k \mathbb{1}_{\bar{\mathcal{B}}_k^{(d)}} + \sum_{i \neq j}^N \mathbb{1}_{\bar{\mathcal{B}}_j^{(d)}} \frac{1}{2} V_N(x_i - x_j) \right) \Psi \rangle\rangle \geq 0. \quad (3.117)$$

Thus, for $\mu > d$, we obtain the bound

$$\tilde{S}_\mu(\Psi, \varphi) = (N-1) \left| \langle\langle \Psi, \mathbb{1}_{\mathcal{B}_1^{(d)}} (1 - p_1 p_2) M_\mu(x_1 - x_2) p_1 p_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \right| \quad (3.118)$$

$$+ \left| \frac{N-1}{2} \langle\langle \Psi, \mathbb{1}_{\mathcal{B}_1^{(d)}} p_1 p_2 M_\mu(x_1 - x_2) p_1 p_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle - \frac{b_{V_N}}{2} \|\varphi^2\|^2 \right| \quad (3.119)$$

$$+ \mathcal{K}(\varphi, A.) N^{1-d+\delta}$$

$$\geq -\tilde{Q}_\mu(\Psi, \varphi).$$

In total, we obtain

$$\epsilon \left(\|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 q_1 \Psi\|^2 + \|\mathbb{1}_{\bar{\mathcal{B}}_1^{(d)}} \mathbb{1}_{\bar{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 \right) \leq |M(\Psi, \varphi)| + |\tilde{S}_\mu(\Psi, \varphi)| + \left| \mathcal{E}_{V_N}(\Psi) - \mathcal{E}_{b_{V_N}}^{GP}(\varphi) \right|.$$

Next, we will estimate $M(\Psi, \varphi)$, $S_\beta(\Psi, \varphi)$ and $\tilde{S}_\mu(\Psi, \varphi)$.

- Estimate of $S_\beta(\Psi, \varphi)$ and $\tilde{S}_\mu(\Psi, \varphi)$.

We first estimate (3.119), using the same estimate as in (3.57). Note that

$$\langle\langle \Psi, \mathbb{1}_{\mathcal{B}_1^{(d)}} p_1 p_2 M_\mu(x_1 - x_2) p_1 p_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle = \langle \varphi, M_\mu \star |\varphi|^2 \varphi \rangle \langle\langle \Psi, \mathbb{1}_{\mathcal{B}_1^{(d)}} p_1 p_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle.$$

Using $\|\mathbf{1}_{\overline{\mathcal{B}}_1^{(d)}}\Psi\| \leq C_\epsilon N^{1-d+\epsilon}$, for any $\epsilon > 0$, (see Lemma 3.3.6 (j)) we obtain, together with $\|p_1 p_2 \Psi\|^2 = 1 - 2\|p_1 q_2 \Psi\|^2 - \|q_1 q_2 \Psi\|^2$

$$\begin{aligned} |(3.119)| &\leq 3\|q_1 \Psi\|^2 + C_\epsilon (N^{1-d+\epsilon} + N^{2-2d+2\epsilon}) + \frac{1}{2}|N\langle \varphi, M_\mu \star |\varphi|^2 \varphi \rangle - N\|M_\mu\|_1 \|\varphi^2\|^2| \\ &\quad + \frac{1}{2}|b_{V_N} - N\|M_\mu\|_1 \|\varphi^2\|^2 + \frac{1}{2}\langle \varphi, M_\mu \star |\varphi|^2 \varphi \rangle|. \end{aligned}$$

Note that, using Young's inequality and (3.57),

$$\begin{aligned} &|\langle \varphi, NM_\mu \star |\varphi|^2 \varphi \rangle - N\|M_\mu\|_1 \|\varphi^2\|^2| \\ &= \left| \int_{\mathbb{R}^2} d^2x |\varphi(x)|^2 (N(M_\mu \star |\varphi|^2)(x) - N\|M_\mu\|_1 |\varphi(x)|^2) \right| \\ &\leq \|\varphi\|_\infty^2 \|N(M_\mu \star |\varphi|^2) - NM_\mu\|_1 \|\varphi^2\|_1 \leq C\|\varphi\|_\infty^2 \|\Delta|\varphi|^2\|_1 N^{-2\mu} \ln(N) \\ &\leq \mathcal{K}(\varphi, A.) N^{-2\mu} \ln(N). \end{aligned}$$

Since $|N\|M_\mu\|_1 - b_{V_N}| \leq C \frac{\ln(N)}{N}$ (see Lemma 3.5.5) and

$$\langle \varphi, M_\mu \star |\varphi|^2 \varphi \rangle \leq \|\varphi\|_\infty^4 \|M_\mu\|_1 \leq C\|\varphi\|_\infty^4 N^{-1},$$

it follows that

$$\begin{aligned} |(3.119)| &\leq \mathcal{K}(\varphi, A.) (\langle \Psi, \widehat{n}^\varphi \Psi \rangle + C_\epsilon (N^{1-d+\epsilon} + N^{2-2d+2\epsilon}) + N^{-2\mu} \ln(N) + N^{-1} \ln(N)) \\ &\leq \mathcal{K}(\varphi, A.) (\langle \Psi, \widehat{n}^\varphi \Psi \rangle + N^{-1} \ln(N)), \end{aligned} \quad (3.120)$$

where the last inequality holds for d large enough (recall that we chose $\mu > d$). Using the same estimates, we obtain

$$(3.113) \leq \mathcal{K}(\varphi, A.) (\langle \Psi, \widehat{n}^\varphi \Psi \rangle + N^{-2\beta} \ln(N) + N^{-1} \ln(N)).$$

Line (3.118) and line (3.112) are controlled by Lemma 3.5.12, which is stated below.

$$(3.112), (3.118) \leq \mathcal{K}(\varphi, A.) (\langle \Psi, \widehat{n} \Psi \rangle + N^{-1/6} \ln(N)).$$

In total, we obtain, for any $\mu > d \geq 1$, the bound

$$\begin{aligned} S_\beta(\Psi, \varphi) &\leq \mathcal{K}(\varphi, A.) (\langle \Psi, \widehat{n} \Psi \rangle + N^{-2\beta} \ln(N) + N^{-1/6} \ln(N)) \\ \tilde{S}_\mu(\Psi, \varphi) &\leq \mathcal{K}(\varphi, A.) (\langle \Psi, \widehat{n} \Psi \rangle + N^{-1/6} \ln(N)). \end{aligned}$$

- Estimate of $M(\Psi, \varphi)$.

First, we estimate (3.104).

$$\begin{aligned} |(3.104)| &\leq 2|\langle \nabla_1 q_1 \Psi, \mathbf{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 p_1 \Psi \rangle| + 2|\langle \nabla_1 q_1 \Psi, \nabla_1 p_1 \Psi \rangle| \\ &\leq 2\|\nabla_1 q_1 \Psi\| \|\mathbf{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 p_1\|_{\text{op}} + 2|\langle \widehat{n}^{-1/2} q_1 \Psi, \Delta_1 p_1 \widehat{n}_1^{1/2} \Psi \rangle|. \end{aligned}$$

By Lemma 3.5.4, we obtain $\|\mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 p_1\|_{\text{op}} \leq C \|\nabla \varphi\|_{\infty} N^{1/2-d}$. Furthermore, we use $\|\nabla_1 q_1 \Psi\| \leq \|\nabla_1 \Psi\| + \|\nabla_1 p_1 \Psi\| \leq \mathcal{K}(\varphi, A.)$ (see also Lemma 3.5.1) and

$$|\langle\langle \widehat{n}^{-1/2} q_1 \Psi, \Delta_1 p_1 \widehat{n}_1^{1/2} \Psi \rangle\rangle| \leq \mathcal{K}(\varphi, A.) \|\widehat{n}_1^{1/2} \Psi\| \|\widehat{n}^{1/2} \Psi\| \leq \mathcal{K}(\varphi, A.) (\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + N^{-1}).$$

Hence, for d large enough,

$$|(3.104)| \leq \mathcal{K}(\varphi, A.) (\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + N^{\frac{1}{2}-d} + N^{-1}) \leq \mathcal{K}(\varphi, A.) (\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + N^{-1}).$$

Line (3.105) is estimated for d large enough, noting that $\|\nabla_1 p_1 \Psi\|^2 = \|\nabla \varphi\|^2 \|p_1 \Psi\|^2$, by

$$\begin{aligned} (3.105) &= \|\mathbb{1}_{\mathcal{A}_1^{(d)}} \nabla_1 p_1 \Psi\|^2 - \|\nabla \varphi\|^2 \\ &\leq |\|\nabla_1 p_1 \Psi\|^2 - \|\nabla \varphi\|^2| + \|\mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 p_1 \Psi\|^2 \\ &\leq C (\|\nabla \varphi\|^2 \langle\langle \Psi, q_1 \Psi \rangle\rangle + \|\nabla \varphi\|_{\infty}^2 N^{1-2d}) \\ &\leq \mathcal{K}(\varphi, A.) (\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + N^{1-2d}). \end{aligned}$$

For line (3.106), we use Lemma 3.5.6 to obtain

$$(3.106) \leq C \|A.\|_{\infty} (\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + N^{-1/2}).$$

In total, we obtain

$$M(\Psi, \varphi) \leq \mathcal{K}(\varphi, A.) (\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + N^{-1/2}).$$

□

Lemma 3.5.11

(a) Let R_{β} and M_{β} be defined as in Lemma 3.3.5. Let V satisfy Assumption 3.2.3. Then, for any $\Psi \in H^1(\mathbb{R}^{2N}, \mathbb{C})$

$$\|\mathbb{1}_{|x_1-x_2| \leq R_{\beta}} \nabla_1 \Psi\|^2 + \frac{1}{2} \langle\langle \Psi, (V_N - M_{\beta})(x_1 - x_2) \Psi \rangle\rangle \geq 0.$$

(b) Let M_{β} be defined as in Lemma 3.3.5. Let $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap H^1(\mathbb{R}^{2N}, \mathbb{C})$. Then, for sufficiently large N and for $\beta > d$,

$$\|\mathbb{1}_{\mathcal{B}_1^{(d)}} \mathbb{1}_{\overline{\mathcal{A}}_1^{(d)}} \nabla_1 \Psi\|^2 + \frac{1}{2} \langle\langle \Psi, \sum_{j=2}^N \mathbb{1}_{\mathcal{B}_1^{(d)}} (V_N - M_{\beta})(x_1 - x_j) \Psi \rangle\rangle \geq 0.$$

Proof:

(a) We first show nonnegativity of the one-particle operator $H^{Z_n} : H^2(\mathbb{R}^2, \mathbb{C}) \rightarrow L^2(\mathbb{R}^2, \mathbb{C})$ given by

$$H^{Z_n} = -\Delta + \frac{1}{2} \sum_{z_k \in Z_n} (V_N(\cdot - z_k) - M_\beta(\cdot - z_k))$$

for any $n \in \mathbb{N}$ and any n -elemental subset $Z_n \subset \mathbb{R}^2$ which is such that the supports of the potentials $M_\beta(\cdot - z_k)$ are pairwise disjoint for any two $z_k \in Z_n$.

Since $f_\beta(\cdot - z_k)$ is the zero energy scattering state of the potential $V_N(\cdot - z_k) - W_\beta(\cdot - z_k)$, it follows that

$$F_\beta^{Z_n} = \prod_{z_k \in Z_n} f_\beta(\cdot - z_k)$$

fulfills $H^{Z_n} F_\beta^{Z_n} = 0$ for any such Z_n . By construction, f_β is a nonnegative function, so is $F_\beta^{Z_n}$. Since $\frac{1}{2} \sum_{z_k \in Z_n} (V_N(\cdot - z_k) - M_\beta(\cdot - z_k)) \in L^\infty(\mathbb{R}^2, \mathbb{C})$, this potential is a infinitesimal perturbation of $-\Delta$, thus $\sigma_{\text{ess}}(H^{Z_n}) = [0, \infty)$. Assume now that H^{Z_n} is not nonnegative. Then, there exists a ground state $\Psi_G \in H^2(\mathbb{R}^2, \mathbb{C})$ of H^{Z_n} of negative energy $E < 0$. The phase of the ground state can be chosen such that the ground state is real and positive (see e.g. Theorem 10.12. in [70]). Since such a ground state of negative energy decays exponentially, that is $\Psi_G(x) \leq C_1 e^{-C_2|x|}$, $C_1, C_2 > 0$, the following scalar product is well defined (although $F_\beta^{Z_n} \notin L^2(\mathbb{R}^2, \mathbb{C})$).

$$\langle F_\beta^{Z_n}, H^{Z_n} \Psi_G \rangle = \langle F_\beta^{Z_n}, E \Psi_G \rangle < 0. \quad (3.121)$$

On the other hand we have since $F_{\beta_1, \beta}^{X_n}$ is the zero energy scattering state

$$\langle F_\beta^{Z_n}, H^{Z_n} \Psi_G \rangle = \langle H^{Z_n} F_\beta^{Z_n}, \Psi_G \rangle = 0.$$

This contradicts (3.121) and the nonnegativity of H^{Z_n} follows.

Now, assume that there exists a $\psi \in H^2(\mathbb{R}^2, \mathbb{C})$ such that the quadratic form

$$Q(\psi) = \|\mathbf{1}_{|\cdot| \leq R_\beta} \nabla \psi\|^2 + \frac{1}{2} \langle \psi, (V_N(\cdot) - M_\beta(\cdot)) \psi \rangle < 0.$$

Since V_N and M_β are spherically symmetric, we can assume that ψ is spherically symmetric. Subsituuting $\psi \rightarrow a\psi$, $a \in \mathbb{R}$, we can furthermore assume that, for all $|x| = R_\beta$, $\psi(x) = 1 - \epsilon$ for $\epsilon > 0$.

Define $\tilde{\psi}$ such that $\tilde{\psi}(x) = \psi(x)$ for $|x| \leq R_\beta$ and $\tilde{\psi}(x) = 1$ for $|x| > R_\beta + \epsilon$ and $\epsilon > 0$. Furthermore, $\tilde{\psi}$ can be constructed such that $\|\mathbf{1}_{|x| \geq R_\beta} \nabla \tilde{\psi}\|^2 \leq C(\epsilon + \epsilon^2)$.

Then $Q(\tilde{\psi}) = Q(\psi) < 0$ holds, because the operator associated with the quadratic form is supported inside the ball $B_0(R_\beta)$.

Using $\tilde{\psi}$, we can construct a set of points Z_n and a $\chi \in H^2(\mathbb{R}^2, \mathbb{C})$ such that $\langle \chi, H^{Z_n} \chi \rangle < 0$, contradicting to nonnegativity of H^{Z_n} .

For $R > 1$ let

$$\xi_R(x) = \begin{cases} R^2/x^2, & \text{for } x > R; \\ 1, & \text{else.} \end{cases}$$

Let now Z_n be a subset $Z_n \subset \mathbb{R}^2$ with $|Z_n| = n$ which is such that the supports of the potentials $W_\beta(\cdot - z_k)$ lie within the sphere around zero with radius R and are pairwise disjoint for any two $z_k \in Z_n$. Since we are in two dimensions we can choose a n which is of order R^2 .

Let now $\chi_R(x) = \xi_R(x) \prod_{z_k \in Z_n} \tilde{\psi}(x - z_k)$. By construction, there exists a $D = \mathcal{O}(1)$ such that $\chi_R(x) = \tilde{\psi}(x - z_k)$ for $|x - z_k| \leq D$. From this, we obtain

$$\begin{aligned} \langle \chi_R, H^{Z_n} \chi_R \rangle &= \|\nabla \chi_R\|^2 + n \frac{1}{2} \langle \psi, (V_N(\cdot) - M_\beta(\cdot)) \psi \rangle \\ &= nQ(\psi) + \sum_{z_k \in Z_n} \|\mathbf{1}_{|x-z_k| \geq R_\beta} \nabla \chi_R\|^2 \\ &\leq nQ(\psi) + Cn(\epsilon + \epsilon^2) + \|\nabla \xi_R\|^2 \\ &= nQ(\psi) + Cn(\epsilon + \epsilon^2) + C. \end{aligned}$$

Choosing R and hence n large enough and ϵ small, we can find a Z_n such that $\langle \chi_R, H^{Z_n} \chi_R \rangle$ is negative, contradicting nonnegativity of H^{Z_n} .

Now, we can prove that

$$\|\mathbf{1}_{|x_1-x_2| \leq R_{\beta_1}} \nabla_1 \Psi\|^2 + \frac{1}{2} \langle \Psi, (V_N - M_\beta)(x_1 - x_2) \Psi \rangle \geq 0. \quad (3.122)$$

holds for any $\Psi \in H^2(\mathbb{R}^{2N}, \mathbb{C})$. Using the coordinate transformation $\tilde{x}_1 = x_1 - x_2, \tilde{x}_i = x_i \forall i \geq 2$, we have $\nabla_{x_1} = \nabla_{\tilde{x}_1}$. Thus (3.122) is equivalent to $\|\mathbf{1}_{|x_1| \leq R_{\beta_1}} \nabla_1 \Psi\|^2 + \frac{1}{2} \langle \Psi, (V_N - M_\beta)(x_1) \Psi \rangle \geq 0 \forall \Psi \in H^2(\mathbb{R}^{2N}, \mathbb{C})$ which follows directly from $Q(\psi) \geq 0$ for all $\psi \in H^2(\mathbb{R}^2, \mathbb{C})$. By a standard density argument, we can conclude that $Q(\Psi) \geq 0 \forall \Psi \in H^1(\mathbb{R}^{2N}, \mathbb{C})$.

(b) Define $c_k = \{(x_1, \dots, x_N) \in \mathbb{R}^{2N} \mid |x_1 - x_k| \leq R_\beta\}$ and $\mathcal{C}_1 = \bigcup_{k=2}^N c_k$. For $(x_1, \dots, x_N) \in \mathcal{B}_1^{(d)}$ it holds that $|x_i - x_j| \geq N^{-d}$ for $2 \leq i, j \leq N$. Let $\beta > d$. Assume that $N^{-d} > 2R_\beta$, which hold for N sufficiently large, since $R_\beta \leq CN^{-\beta}$. Then, it follows that, for $2 \leq i, j \leq N$ and $i \neq j$, $(c_i \cap \mathcal{B}_1^{(d)}) \cap (c_j \cap \mathcal{B}_1^{(d)}) = \emptyset$. Under the same conditions, we also have $\mathbf{1}_{\overline{\mathcal{A}}_1^{(d)}} \geq \mathbf{1}_{\mathcal{C}_1}$. Therefore,

$$\mathbf{1}_{\overline{\mathcal{A}}_1^{(d)}} \mathbf{1}_{\mathcal{B}_1^{(d)}} \geq \mathbf{1}_{\mathcal{C}_1} \mathbf{1}_{\mathcal{B}_1^{(d)}} = \mathbf{1}_{\mathcal{C}_1 \cap \mathcal{B}_1^{(d)}} = \mathbf{1}_{\bigcup_{k=2}^N (c_k \cap \mathcal{B}_1^{(d)})} = \sum_{k=2}^N \mathbf{1}_{c_k \cap \mathcal{B}_1^{(d)}} = \mathbf{1}_{\mathcal{B}_1^{(d)}} \sum_{k=2}^N \mathbf{1}_{c_k}.$$

Note that $\mathbf{1}_{\mathcal{B}_1^{(d)}}$ depends only on x_2, \dots, x_N . By this

$$\|\mathbf{1}_{\overline{\mathcal{A}}_1^{(d)}} \mathbf{1}_{\mathcal{B}_1^{(d)}} \nabla_1 \Psi\|^2 \geq \sum_{k=2}^N \|\mathbf{1}_{c_k} \nabla_1 \mathbf{1}_{\mathcal{B}_1^{(d)}} \Psi\|^2 = (N-1) \|\mathbf{1}_{|x_1-x_2| \leq R_\beta} \nabla_1 \mathbf{1}_{\mathcal{B}_1^{(d)}} \Psi\|^2.$$

This yields

$$(3.115) \geq (N-1) \left(\|\mathbb{1}_{|x_1-x_2| \leq R_\beta} \nabla_1 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi\|^2 + \frac{1}{2} \langle\langle \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi, (V_N - M_\beta)(x_1 - x_2) \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \right) \geq 0.$$

where the last inequality follows from (a)

□

Lemma 3.5.12 *Let $W_\beta \in \mathcal{V}_\beta$ as in Definition 3.3.4. Let $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap H^1(\mathbb{R}^{2N}, \mathbb{C})$ and $\|\nabla_1 \Psi\|$ be bounded uniformly in N . Let d in Definition 3.5.4 of $\mathbb{1}_{\mathcal{B}_1^{(d)}}$ sufficiently large. Let $\Gamma \in \{\Psi, \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi\}$. Then, for all $\beta > 0$,*

(a)

$$N |\langle\langle \Gamma, q_1 p_2 W_\beta(x_1 - x_2) p_1 p_2 \Gamma \rangle\rangle| \leq C \|\varphi\|_\infty^2 \langle\langle \Psi, \hat{n} \Psi \rangle\rangle.$$

(b)

$$N |\langle\langle \Gamma, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \Gamma \rangle\rangle| \leq \mathcal{K}(\varphi, A.) (\langle\langle \Psi, \hat{n} \Psi \rangle\rangle + N^{-1/6} \ln(N)).$$

(c)

$$N |\langle\langle \Gamma, (1 - p_1 p_2) W_\beta(x_1 - x_2) p_1 p_2 \Gamma \rangle\rangle| \leq \mathcal{K}(\varphi, A.) (\langle\langle \Psi, \hat{n} \Psi \rangle\rangle + N^{-1/6} \ln(N)).$$

Proof:

(a) Let first $\Gamma = \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi$. Then,

$$N \left| \langle\langle \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi, q_1 p_2 W_\beta(x_1 - x_2) p_1 p_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \right| \quad (3.123)$$

$$\leq N \left| \langle\langle \mathbb{1}_{\overline{\mathcal{B}}_1^{(d)}} \Psi, q_1 p_2 W_\beta(x_1 - x_2) p_1 p_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \right| \quad (3.123)$$

$$+ N \left| \langle\langle \Psi, q_1 p_2 W_\beta(x_1 - x_2) p_1 p_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \right|. \quad (3.124)$$

Using Lemma 3.5.5 together with $\|p_2 W_\beta(x_1 - x_2) p_2\|_{\text{op}} \leq \|\varphi\|_\infty^2 \|W_\beta\|_1$, the first line can be bounded, for any $\epsilon > 0$, by

$$(3.123) \leq \mathcal{K}(\varphi, A.) N \|\mathbb{1}_{\overline{\mathcal{B}}_1^{(d)}} \Psi\| \|W_\beta\|_1 \leq \mathcal{K}(\varphi, A.) N^{1-d+\epsilon}. \quad (3.125)$$

The second term is bounded by

$$\begin{aligned}
(3.124) &= N \left| \langle\langle \sqrt{|W_\beta(x_1 - x_2)|} q_1 p_2 (\hat{n})^{-\frac{1}{2}} \Psi, \sqrt{|W_\beta(x_1 - x_2)|} p_1 p_2 \hat{n}_1^{\frac{1}{2}} \mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi \rangle\rangle \right| \\
&\leq C N \|\sqrt{|W_\beta(x_1 - x_2)|} p_2\|_{\text{op}}^2 \left(\|q_1 (\hat{n})^{-\frac{1}{2}} \Psi\|^2 + \|\hat{n}_1^{\frac{1}{2}} \mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi\|^2 \right) \\
&\leq C N \|\sqrt{|W_\beta(x_1 - x_2)|} p_2\|_{\text{op}}^2 \left(\langle\langle \Psi, \hat{n} \Psi \rangle\rangle + \|\hat{n}_1^{\frac{1}{2}} \Psi\|^2 + \|\hat{n}_1^{\frac{1}{2}} \mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi\|^2 \right) \\
&\leq C N \|W_\beta\|_1 \|\varphi\|_\infty^2 \left(\langle\langle \Psi, \hat{n} \Psi \rangle\rangle + \|\mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi\|^2 \right) \\
&\leq C \|\varphi\|_\infty^2 (\langle\langle \Psi, \hat{n} \Psi \rangle\rangle + N^{1-d+\epsilon}).
\end{aligned}$$

Choosing d large enough, $N^{1-d+\epsilon}$ is smaller than $\langle\langle \Psi, \hat{n} \Psi \rangle\rangle$. This yields (a) in the case $\Gamma = \mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi$. The inequality (a) can be proven analogously for $\Gamma = \Psi$.

(b) Let $\Gamma = \mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi$. We first consider (b) for potentials with $\beta < 1/4$. We have to estimate

$$\begin{aligned}
N |\langle\langle \mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi \rangle\rangle| &\leq N |\langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \Psi \rangle\rangle| \\
&+ N |\langle\langle \mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \Psi \rangle\rangle| + N |\langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi \rangle\rangle| \\
&+ N |\langle\langle \mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi \rangle\rangle| \\
&\leq N |\langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \Psi \rangle\rangle| \\
&+ C N \|\mathbb{1}_{\mathcal{B}^{(d)}_1} \Psi\| \|W_\beta\|_\infty. \tag{3.126}
\end{aligned}$$

The last term is bounded, for any $\epsilon > 0$, by

$$(3.127) \leq C_\epsilon N N^{1-d+\epsilon} N^{-1+2\beta} \leq N^{-2},$$

where the last inequality holds choosing d large enough.

Using Lemma 2.0.5 (c) and Lemma 2.0.10 with $O_{1,2} = q_2 W_\beta(x_1 - x_2) p_2$, $\Omega = N^{-1/2} q_1 \Psi$ and $\chi = N^{1/2} p_1 \Psi$ we get

$$\begin{aligned}
(3.126) &\leq \|q_1 \Psi\|^2 + N^2 |\langle\langle q_2 \Psi, p_1 \|\sqrt{|W_\beta(x_1 - x_2)|} p_3 \|\sqrt{|W_\beta(x_1 - x_3)|} \\
&\quad \times \|\sqrt{|W_\beta(x_1 - x_2)|} p_2 \|\sqrt{|W_\beta(x_1 - x_3)|} p_1 q_3 \Psi \rangle\rangle| \\
&\quad + N^2 (N-1)^{-1} \|q_2 W_\beta(x_1 - x_2) p_2 p_1 \Psi\|^2 \\
&\leq \|q_1 \Psi\|^2 + N^2 \|\|\sqrt{|W_\beta(x_1 - x_2)|} p_1\|_{\text{op}}^4 \|q_2 \Psi\|^2 \\
&\quad + C N \|W_\beta(x_1 - x_2) p_2\|_{\text{op}}^2.
\end{aligned}$$

With Lemma 2.0.5 (e) we get the bound

$$(3.126) \leq \|q_1 \Psi\|^2 + N^2 \|\varphi\|_\infty^4 \|W_\beta\|_1^2 \|q_1 \Psi\|^2 + C N \|W_\beta\|^2 \|\varphi\|_\infty^2.$$

Note, that $\|W_\beta\|_1 \leq CN^{-1}$, $\|W_\beta\|^2 \leq CN^{-2+2\beta}$ Hence

$$(3.126) \leq C (\langle\langle \Psi, q_1 \Psi \rangle\rangle + \mathcal{K}(\varphi) N^{-1+2\beta}).$$

Note that, for $\beta < 1/4$, $N^{-1+2\beta} \leq N^{-1/6} \ln(N)$. Using the same bounds for $\Gamma = \Psi$, we obtain (b) for the case $\beta < 1/4$.

b) for $1/4 \leq \beta$:

We use $U_{\beta_1, \beta}$ from Definition 3.5.2 for some $0 < \beta_1 < 1/4$.

$Z_\beta^\varphi(x_1, x_2) - W_\beta + U_{\beta_1, \beta}$ has the form of $Z_{\beta_1}^\varphi(x_1, x_2)$ which has been controlled above. It is left to control

$$N \left| \langle\langle \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi, p_1 p_2 (W_\beta(x_1 - x_2) - U_{\beta_1, \beta}(x_1 - x_2)) q_1 q_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \right|.$$

Let $\Delta h_{\beta_1, \beta} = W_\beta - U_{\beta_1, \beta}$. Integrating by parts and using that $\nabla_1 h_{\beta_1, \beta}(x_1 - x_2) = -\nabla_2 h_{\beta_1, \beta}(x_1 - x_2)$ gives

$$\begin{aligned} & N \left| \langle\langle \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi, p_1 p_2 (W_\beta(x_1 - x_2) - U_{\beta_1, \beta}(x_1 - x_2)) q_1 q_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \right| \\ &= N \left| \langle\langle \nabla_1 p_1 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi, p_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) q_1 q_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \right| \end{aligned} \quad (3.128)$$

$$+ N \left| \langle\langle \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi, p_1 p_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) \nabla_1 q_1 q_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \right|. \quad (3.129)$$

Let $(a_1, b_1) = (q_1, \nabla p_1)$ or $(a_1, b_1) = (\nabla q_1, p_1)$. Then, both terms can be estimated as follows:

We use Lemma 2.0.10 with $\Omega = N^{-\eta/2} a_1 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi$, $O_{1,2} = N^{1+\eta/2} q_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) p_2$ and $\chi = b_1 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi$. We choose $\eta < 2\beta_1$.

$$\begin{aligned} & N \left| \langle\langle \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi, a_1 p_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) b_1 q_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \right| \\ & \leq N^{-\eta} \|a_1 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi\|^2 \end{aligned} \quad (3.130)$$

$$+ \frac{N^{2+\eta}}{N-1} \|q_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) b_1 p_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi\|^2 \quad (3.131)$$

$$+ N^{2+\eta} \left| \langle\langle \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi, b_1 p_2 q_3 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) \nabla_3 h_{\beta_1, \beta}(x_1 - x_3) b_1 q_2 p_3 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle\rangle \right|^{1/2}. \quad (3.132)$$

We obtain (note that $\mathbb{1}_{\mathcal{B}_1^{(d)}}$ does not depend on x_1)

$$(3.130) \leq N^{-\eta} \|a_1 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi\|^2 = N^{-\eta} \|\mathbb{1}_{\mathcal{B}_1^{(d)}} a_1 \Psi\|^2 \leq \mathcal{K}(\varphi, A) N^{-\eta}.$$

since both $\|\nabla q_1 \Psi\|$ and $\|q_1 \Psi\|$ are bounded uniformly in N . Since q_2 is a projector it follows that

$$\begin{aligned}
 (3.131) \leq & \frac{N^{2+\eta}}{N-1} \|\nabla_2 h_{\beta_1, \beta}(x_1 - x_2) p_2\|_{\text{op}}^2 \|b_1 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi\|^2 \\
 \leq & C \frac{N^{2+\eta}}{N-1} \|\varphi\|_\infty^2 \|\nabla h_{\beta_1, \beta}\|^2 \|b_1 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi\|^2 \\
 \leq & \mathcal{K}(\varphi, A.) N^{\eta-1} \ln(N) \|\varphi\|_\infty^2,
 \end{aligned}$$

where we used Lemma 3.5.3 in the last step.

Next, we estimate

$$\begin{aligned}
 (3.132) \leq & N^{2+\eta} \|p_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) b_1 q_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi\|^2 \\
 \leq & 2N^{2+\eta} \|p_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) b_1 q_2 \mathbb{1}_{\overline{\mathcal{B}}_1^{(d)}} \Psi\|^2
 \end{aligned} \tag{3.133}$$

$$+ 2N^{2+\eta} \|p_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) b_1 q_2 \Psi\|^2. \tag{3.134}$$

The first term can be estimated as

$$\begin{aligned}
 (3.133) \leq & C N^{2+\eta} \|\nabla_2 h_{\beta_1, \beta}(x_1 - x_2) b_1\|_{\text{op}}^2 \|\mathbb{1}_{\overline{\mathcal{B}}_1^{(d)}} \Psi\|^2 \\
 \leq & C N^{2+\eta} \|\nabla_2 h_{\beta_1, \beta}\|^2 (\|\varphi\|_\infty^2 + \|\nabla \varphi\|_\infty^2) \|\mathbb{1}_{\overline{\mathcal{B}}_1^{(d)}} \Psi\|^2 \\
 \leq & \mathcal{K}(\varphi, A.) N^{2+\eta} N^{-2} \ln(N) N^{2-2d+2\epsilon} = \mathcal{K}(\varphi, A.) N^{2-2d+2\epsilon+\eta} \ln(N),
 \end{aligned}$$

for any $\epsilon > 0$. For d large enough, this term is subleading. The last term can be estimated as

$$\begin{aligned}
 (3.134) \leq & 2N^{2+\eta} \|p_2 h_{\beta_1, \beta}(x_1 - x_2) b_1 \nabla_2 q_2 \Psi\|^2 \\
 & + 2N^{2+\eta} \|\langle \varphi(x_2) \rangle \langle \nabla \varphi(x_2) | h_{\beta_1, \beta}(x_1 - x_2) b_1 q_2 \Psi \rangle\|^2 \\
 \leq & C N^{2+\eta} \|p_2 h_{\beta_1, \beta}(x_1 - x_2)\|_{\text{op}}^2 \|b_1 \nabla_2 q_2 \Psi\|^2 \\
 & + C N^{2+\eta} \|\langle \varphi(x_2) \rangle \langle \nabla \varphi(x_2) | h_{\beta_1, \beta}(x_1 - x_2) \rangle\|_{\text{op}}^2 \|b_1 q_2 \Psi\|^2 \\
 \leq & C N^{2+\eta} (\|\nabla \varphi\|_\infty^2 + \|\varphi\|_\infty^2) \|h_{\beta_1, \beta}\|^2 (1 + \|\nabla \varphi\|^2) \\
 \leq & \mathcal{K}(\varphi, A.) N^{\eta-2\beta_1} \ln(N)^2.
 \end{aligned}$$

Combining both estimates we obtain, for any $\beta > 1$,

$$\begin{aligned}
 N \left| \langle \langle \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \mathbb{1}_{\mathcal{B}_1^{(d)}} \Psi \rangle \rangle \right| \\
 \leq \inf_{\eta > 0} \inf_{0 < \mu < 1/4} (\mathcal{K}(\varphi, A.) (\langle \langle \Psi, \widehat{n} \Psi \rangle \rangle + N^{-1+2\mu} + N^{-\eta} + N^{\eta-1} \ln(N) + N^{\eta-2\mu} \ln(N))) \\
 \leq \mathcal{K}(\varphi, A.) (\langle \langle \Psi, \widehat{n} \Psi \rangle \rangle + N^{-1/6} \ln(N)).
 \end{aligned}$$

where the last inequality comes from choosing $\eta = 1/3$ and $\mu = 1/4$. For $\Gamma = \Psi$, (b) can be estimated the same way, yielding the same bound.

(c) This follows from (a) and (b), using that $1 - p_1 p_2 = q_1 q_2 + p_1 q_2 + q_1 p_2$. □

3.6 Regularity of the solution φ_t

In our estimates, we need the regularity conditions

$$\|\nabla \varphi_t\|_\infty < \infty, \quad \|\varphi_t\|_\infty < \infty, \quad \|\nabla \varphi_t\| < \infty, \quad \|\Delta \varphi_t\| < \infty.$$

That is, we need $\varphi_t \in H^2(\mathbb{R}^2, \mathbb{C}) \cap W^{1,\infty}(\mathbb{R}^2, \mathbb{C})$. Then, $\|\Delta |\varphi_t|^2\|$, $\|\Delta |\varphi_t|^2\|_1$ and $\|\varphi_t^2\|$, which also appear in our estimates, can be bounded by

$$\begin{aligned} \Delta |\varphi_t|^2 &= \varphi_t^* \Delta \varphi_t + \varphi_t \Delta \varphi_t^* + 2(\nabla \varphi_t^*) \cdot (\nabla \varphi_t) \\ \|\Delta |\varphi_t|^2\| &\leq 2\|\Delta \varphi_t\| \|\varphi_t\|_\infty + 2\|\nabla \varphi_t\| \|\nabla \varphi_t\|_\infty \\ \|\Delta |\varphi_t|^2\|_1 &\leq 4\|\Delta \varphi_t\| \\ \|\varphi_t^2\| &\leq \|\varphi_t\|_\infty \|\varphi_t\|. \end{aligned}$$

Recall the Sobolev embedding Theorem, which implies in particular $H^k(\mathbb{R}^2, \mathbb{C}) = W^{k,2}(\mathbb{R}^2, \mathbb{C}) \subset C^{k-2}(\mathbb{R}^2, \mathbb{C})$. If $\varphi \in C^1(\mathbb{R}^2, \mathbb{C}) \cap H^1(\mathbb{R}^2, \mathbb{C})$, then $\varphi \in W^{1,\infty}(\mathbb{R}^2, \mathbb{C})$ follows since both φ and $\nabla \varphi$ have to decay at infinity. Thus, $\varphi_t \in H^3(\mathbb{R}^2, \mathbb{C})$ implies $\varphi_t \in H^2(\mathbb{R}^2, \mathbb{C}) \cap W^{1,\infty}(\mathbb{R}^2, \mathbb{C})$, which suffices for our estimates. Since φ_t obeys a defocusing nonlinear Schrödinger equation, we expect the regularity of the solution φ_t to follow from the regularity of the initial datum φ_0 . For a certain class of external potentials A_t this has been proven in [11]:

Lemma 3.6.1 *Let $\varphi_0 \in \Sigma^k(\mathbb{R}^2, \mathbb{C}) = \{f \in L^2(\mathbb{R}^2, \mathbb{C}) \mid \sum_{\alpha+\beta \leq k} \|x^\alpha \partial_x^\beta f\| < \infty\}$, for $k \geq 2$. Let, for $b > 0$, φ_t the unique solution to*

$$i\partial_t \varphi_t = (-\Delta + A_t + b|\varphi_t|^2)\varphi_t.$$

Let $A_t \in L_{loc}^\infty(\mathbb{R}_t \times \mathbb{R}_x^2, \mathbb{C})$ real valued and smooth with respect to the space variable: for (almost) all $t \in \mathbb{R}$, the map $x \mapsto A_t(x)$ is C^∞ . Moreover, A_t is at most quadratic in space, uniformly w.r.t. time t :

$$\forall \alpha \in \mathbb{N}^2, |\alpha| \geq 2, \quad \partial_x^\alpha A_t \in L^\infty(\mathbb{R}_t \times \mathbb{R}_x^d, \mathbb{C}).$$

In addition, $t \mapsto \sup_{|x| \leq 1} |A_t(x)|$ belongs to $L^\infty(\mathbb{R}, \mathbb{C})$. Then

(a) $\varphi_t \in \Sigma^k(\mathbb{R}^2, \mathbb{C})$, which implies $\varphi_t \in H^k(\mathbb{R}^2, \mathbb{C})$.

(b) $\|\varphi_t\| = \|\varphi_0\|$.

(c) *Let $\varphi_0 \in \Sigma^3(\mathbb{R}^2, \mathbb{C})$. Assume in addition that $\|A_t\|_\infty < \infty$ and $\|\dot{A}_t\|_\infty < \infty$. Then, for any fixed $t \geq 0$, $\mathcal{K}(\varphi_t, A_t) < \infty$ follows.*

Proof: Part (a) is Corollary 1.4. in [11]. We like to remark that $\|\varphi_t\|_{H^k} \leq C$ holds, if $A_t = 0$, see Section 1.2. in [11]. The conditions on A_t are for example satisfied if $A_t \in C_c^\infty(\mathbb{R}^2, \mathbb{R})$ for all $t \in \mathbb{R}$, $A_t(x) = 0$, for all $|t| \geq T$. Part (b) can be verified directly, using the existence of global in time solutions. Part (c) follows from (a) and the embedding $H^3(\mathbb{R}^2, \mathbb{C}) \subset H^2(\mathbb{R}^2, \mathbb{C}) \cap W^{1,\infty}(\mathbb{R}^2, \mathbb{C})$.

□

Chapter 4

Derivation of the Gross-Pitaevskii Equation for a Class of Non Purely Positive Potentials

Contributions of the author and Acknowledgments

This chapter presents joint work with Prof. Dr. Peter Pickl and has with minor modifications already been published as the preprint [27]. In this chapter, parts of the proofs have been adapted to also cover two dimensions. The preprint was written by me. My contribution to the conceptual ideas is 70 % and my share on their technical implementation is 80 %.

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4.1 Introduction

In this chapter, we will analyze the dynamics of a Bose-Einstein condensate in the Gross-Pitaevskii regime for interactions V which need not to be nonnegative, but may have an attractive part. The theorem we are going to present generalizes the derivation of the Gross-Pitaevskii equation in three dimensions as conducted in [60].

Let us first define the N -body quantum problem we want to study. The evolution of N interacting bosons is described by a time-dependent wave-function $\Psi_t \in L_s^2(\mathbb{R}^{3N}, \mathbb{C})$, $\|\Psi_t\| = 1$. Assuming in addition $\Psi_0 \in H^2(\mathbb{R}^{3N}, \mathbb{C})$, the evolution of Ψ_t is then described by the N -particle Schrödinger equation

$$i\partial_t \Psi_t = H\Psi_t. \quad (4.1)$$

The time-dependent Hamiltonian H we will study is defined by

$$H = - \sum_{j=1}^N \Delta_j + N^2 \sum_{1 \leq j < k \leq N} V(N(x_j - x_k)) + \sum_{j=1}^N A_t(x_j). \quad (4.2)$$

In the following, we assume $A_t \in L^\infty(\mathbb{R}^3, \mathbb{R})$ and $V \in L_c^\infty(\mathbb{R}^3, \mathbb{R})$, V spherically symmetric. We will also use the common notation $V_1(x) = N^2 V(Nx)$. More generally, one can study the properties of Bose gases for a larger class of scaling parameters $0 \leq \beta \leq 1$, setting $V_\beta(x) = N^{-1+3\beta} V(N^\beta x)$. For $0 < \beta \leq 1$ and large particle number N , the potential gets δ -like, which indicates that the mathematical description may become more involved the bigger β is chosen. The so-called Gross-Pitaevskii regime $\beta = 1$ is special, since then the two-particle correlations play a crucial role for the dynamics, see Section 4.3.1 and also Chapter 3 for the discussion of the two-dimensional Gross-Pitaevskii equation.

We will derive an approximate solution of (4.1) in the trace class topology of reduced density matrices. Recall the definition of the one particle reduced density matrix $\gamma_{\Psi_0}^{(1)}$ given by the integral kernel

$$\gamma_{\Psi_0}^{(1)}(x, x') = \int_{\mathbb{R}^{3N-3}} \Psi_0^*(x, x_2, \dots, x_N) \Psi_0(x', x_2, \dots, x_N) d^3 x_2 \dots d^3 x_N. \quad (4.3)$$

To account for the physical situation of a Bose-Einstein condensate, we assume complete condensation in the limit of large particle number N . This amounts to assume that, for $N \rightarrow \infty$, $\gamma_{\Psi_0}^{(1)} \rightarrow |\varphi_0\rangle\langle\varphi_0|$ in trace norm for some $\varphi_0 \in L^2(\mathbb{R}^3, \mathbb{C})$, $\|\varphi_0\| = 1$. Our main goal is to show the persistence of condensation over time. Let a denote the scattering length of the potential $\frac{1}{2}V$ (see Section 4.3.1 for the precise definition of a) and let φ_t solve the nonlinear Gross-Pitaevskii equation

$$i\partial_t \varphi_t = (-\Delta + A_t) \varphi_t + 8\pi a |\varphi_t|^2 \varphi_t =: h^{\text{GP}} \varphi_t \quad (4.4)$$

with initial datum φ_0 (we assume $\varphi_t \in H^2(\mathbb{R}^3, \mathbb{C})$, see below). We then prove that the time evolved reduced density matrix $\gamma_{\Psi_t}^{(1)}$ converges to $|\varphi_t\rangle\langle\varphi_t|$ in trace norm as $N \rightarrow \infty$ with convergence rate of order $N^{-\eta}$ for some $\eta > 0$.

The rigorous derivation of effective evolution equations has a long history, see e.g. [2, 4, 5, 7, 8, 9, 14, 17, 18, 19, 20, 25, 26, 30, 31, 32, 34, 49, 50, 51, 53, 54, 55, 59, 60, 61, 65] and references therein. The derivation of the three dimensional time-dependent Gross-Pitaevskii equation for nonnegative potentials was first conducted in [19]. Afterward, this result has been improved by [4, 5, 49, 60]. The ground state properties of dilute Bose gases were treated in [6, 45, 46, 47, 43, 42, 57, 64, 72], see also the monograph [41] and references therein.

As mentioned previously, we will generalize the result presented in [60] to a specific class of interactions V which are not assumed to be nonnegative everywhere. Let us stress that persistence of condensation is not expected for arbitrary V . For strongly attractive potentials, even a small fraction of particles which leave the condensate over time may cluster, subsequently causing the condensate to collapse in finite time. The dynamical collapse of a

Bose gas under such circumstances is well known within the physical community and was mathematically treated in [50]. The breakdown of condensation has also been observed in experiments [21]. Consequently, the result we are going to prove can only be valid under certain restrictions on V . The class of potentials we consider is chosen such that V has a repulsive core, i.e. there exists a $r_1 > 0$, such that $V(x) \geq \lambda^+$, for some $\lambda^+ > 0$ and for all $|x| \leq r_1$. This condition prevents clustering of particles. If furthermore the negative part of V fulfills some restrictions (see Assumption 4.2.3), a result by Jun Yin [72] then implies that the Hamiltonian we consider in this note is stable of second kind. The author proves in particular that for such potentials the ground state energy per particle of a dilute, homogeneous Bose gas is at first order given by the well-known formula $4\pi a\rho N$. Among the steps of the proof in [72], it is shown that the Hamiltonian (4.2) -without external potential A_t - restricted to configurations where at least three particles are close to each other is a nonnegative operator. We will adapt this non-trivial operator inequality in our proof to control the kinetic energy of those particles which leave the condensate, see Lemma 4.3.21. We like to remark that the Assumptions 4.2.3 on V stated below imply that the scattering length a of the potential $\frac{1}{2}V$ is nonnegative. Consequently, the effective Gross-Pitaevskii dynamics (4.4) is repulsive, which reflects the fact that the condensate is stable.

The result presented in [72] implies further that there exists an $\epsilon > 0$, such that

$$-\epsilon \sum_{k=1}^N \Delta_k \leq -\sum_{k=1}^N \Delta_k + \sum_{i < j} V_1(x_i - x_j), \quad (4.5)$$

$$\epsilon \sum_{i < j} |V_1(x_i - x_j)| \leq -\sum_{k=1}^N \Delta_k + \sum_{i < j} V_1(x_i - x_j). \quad (4.6)$$

The first operator inequality bounds $\|\nabla_1 \Psi_t\|$ uniformly in N , if initially the energy per particle is of order 1. If the kinetic energy were not uniformly bounded, one cannot expect condensation, see e.g. [50] for a nice discussion. Under the same assumption, the second inequality (4.6) implies $\|V_1(x_1 - x_2)\Psi_t\| \leq N^{1/2}$, see Lemma 4.3.17. These two inequalities are crucial in our proof to control the rate of particles which leave the condensate over time and thus to extend the result presented in [60].

4.2 Main Result

Notation 4.2.1 *During the rest of this chapter, a will always denote the scattering length of the potential $\frac{1}{2}V$, as defined in Section 4.3.1.*

Define the energy functional $\mathcal{E} : H^2(\mathbb{R}^{3N}, \mathbb{C}) \rightarrow \mathbb{R}$

$$\mathcal{E}(\Psi) = N^{-1} \langle \langle \Psi, H\Psi \rangle \rangle, \quad (4.7)$$

as well as the Gross-Pitaevskii energy functional $\mathcal{E}^{GP} : H^2(\mathbb{R}^3, \mathbb{C}) \rightarrow \mathbb{R}$

$$\mathcal{E}^{GP}(\varphi) := \langle \nabla \varphi, \nabla \varphi \rangle + \langle \varphi, (A_t + 4\pi a|\varphi|^2)\varphi \rangle = \langle \varphi, (h^{GP} - 4\pi a|\varphi|^2)\varphi \rangle. \quad (4.8)$$

Next, we will define the class of interaction potentials V we will consider. This class is essentially the one considered in [72], Theorem 2; see also Corollary 1 and Corollary 2 in [72] for a different characterization of the class of potentials V . Here, we require in addition that the potential changes its sign only once. This facilitates the discussion of the scattering state, see Section 4.3.1. In principle, one could ease this additional assumption by generalizing the proofs given in Section 4.3.1. We will state several lemmata and definitions below for both two and three dimensions. The two dimensional lemmata are used in Chapter 3 to prove the validity of the two dimensional Gross-Pitaevskii equation for potentials which may have an attractive part.

Definition 4.2.2 *Let $d \in \{2, 3\}$ and let $B_r(x) = \{z \in \mathbb{R}^d \mid |x - z| < r\}$ and divide \mathbb{R}^d into cubes (or rectangles, for $d = 2$, respectively) C_n , $n \in \mathbb{Z}$ of side length b_1/\sqrt{d} ; that is $\mathbb{R}^d = \bigcup_{n=-\infty}^{\infty} C_n$. Furthermore, assume that $\overset{\circ}{C}_n \cap \overset{\circ}{C}_m = \emptyset$ for $m \neq n$. Define*

$$n(b_1, b_2) = \max_{x \in \mathbb{R}^d} \#\{n : C_n \cap B_{b_2}(x) \neq \emptyset\}.$$

Thus, $n(b_1, b_2)$ gives the maximal number of cubes (or rectangles) with side length b_1/\sqrt{d} one needs to cover a sphere with radius b_2 .

Assumption 4.2.3 *Let $d \in \{2, 3\}$ and let $V \in L_c^\infty(\mathbb{R}^d, \mathbb{R})$ spherically symmetric and let $V(x) = V^+(x) - V^-(x)$, where $V^+, V^- \in L_c^\infty(\mathbb{R}^d, \mathbb{R})$ are spherically symmetric, such that $V^+(x), V^-(x) \geq 0$ and the supports of V^+ and V^- are disjoint. Assume that*

- (a) *Let $R > r_2 > 0$ and assume $\text{supp}(V^+) \in B_{r_2}(0)$, as well as $\text{supp}(V^-) \in B_R(0) \setminus B_{r_2}(0)$.*
- (b) *There exists $\lambda^+ > 0$ and $r_1 > 0$, such that $V^+(x) \geq \lambda^+$ for all $x \in B_{r_1}(0)$.*
- (c) *Define $\lambda^- = \|V^-\|_\infty$, as well as $n_1 = n(r_1, R)$ and $n_2 = n(r_1, 3R)$. Define, for $0 < \epsilon < 1$,*

$$\mathcal{E}_R(\varphi) = \int_{B_R(0)} \left(|\nabla_x \varphi(x)|^2 + \frac{1}{1-\epsilon} n_1 (2V^+(x) - 4V^-(x)) |\varphi(x)|^2 \right) d^d x. \quad (4.9)$$

We then assume that for some $0 < \epsilon < 1$

$$\inf_{\varphi \in C^1(\mathbb{R}^d, \mathbb{C}), \varphi(R)=1} (\mathcal{E}_R(\varphi)) \geq 0, \quad (4.10)$$

$$\lambda^+ > 8n_2\lambda^-. \quad (4.11)$$

Notation 4.2.4 *We will use the constants $r_1, r_2, R, \lambda^+, \lambda^-$, as well as n_1, n_2 throughout this chapter as defined above.*

Remark 4.2.5 Condition (4.10) implies $a \geq 0$, see Theorem C.1.,(C.8.) in [41]. Assumption 4.2.3 implies that there exists $\epsilon > 0, \mu > 0$ such that

$$-\sum_{k=1}^N \Delta_k + \sum_{i < j=1}^N (V_1^+(x_i - x_j) - (1 + \epsilon)V_1^-(x_i - x_j)) \geq 0, \quad (4.12)$$

$$-(1 - \mu) \sum_{k=1}^N \Delta_k + \sum_{i < j=1}^N V_1(x_i - x_j) \geq 0, \quad (4.13)$$

see Lemma 4.3.10 and Corollary 4.3.15. The Inequality (4.12) can only hold for $a \geq 0$, see [67] and is thus in accordance with Condition (4.10). Thus, although the potential V may have an attractive part V^- , the effective Gross-Pitaevskii Equation (4.4) is repulsive.

It also follows from Assumption 4.2.3 (c)

$$-\Delta + \frac{1}{2}V \geq 0. \quad (4.14)$$

We now state the main Theorem:

Theorem 4.2.6 Let $\Psi_0 \in L_s^2(\mathbb{R}^{3N}, \mathbb{C}) \cap H^2(\mathbb{R}^{3N}, \mathbb{C})$ with $\|\Psi_0\| = 1$. Let $\varphi_0 \in H^2(\mathbb{R}^3, \mathbb{C})$ with $\|\varphi_0\| = 1$. Let $\lim_{N \rightarrow \infty} \text{Tr}|\gamma_{\Psi_0}^{(1)} - |\varphi_0\rangle\langle\varphi_0|| = 0$, as well as $\lim_{N \rightarrow \infty} \mathcal{E}(\Psi_0) = \mathcal{E}^{GP}(\varphi_0)$. Let Ψ_t the unique solution to $i\partial_t \Psi_t = H\Psi_t$ with initial datum Ψ_0 and assume that V fulfills Assumption 4.2.3. Let φ_t the unique solution to $i\partial_t \varphi_t = h^{GP}\varphi_t$ with initial datum φ_0 and assume $\varphi_t \in H^2(\mathbb{R}^3, \mathbb{C})$. Let the external potential A_t fulfill $A_t \in C^1(\mathbb{R}^3, L^\infty(\mathbb{R}^3, \mathbb{R}))$. Then,

(a) for any $t > 0$

$$\lim_{N \rightarrow \infty} \mu_1^{\Psi_t} = |\varphi_t\rangle\langle\varphi_t| \quad (4.15)$$

in operator norm.

(b) if $\int_0^\infty (\|\varphi_s\|_\infty + \|\nabla \varphi_s\|_{6,loc} + \|\dot{A}_s\|_\infty) ds < \infty$ where $\|\cdot\|_{6,loc} : L^2(\mathbb{R}^2, \mathbb{C}) \rightarrow \mathbb{R}^+$ is the “local L^6 -norm” given by

$$\|\varphi\|_{6,loc} := \sup_{x \in \mathbb{R}^3} \|\mathbb{1}_{|\cdot-x| \leq 1} \varphi\|_6,$$

then the convergence (4.15) is uniform in $t > 0$.

Remark 4.2.7 (a) For potentials V which satisfy Assumption 4.2.3, convergence of the ground state energies $\mathcal{E}(\Psi^{gs}) - \mathcal{E}^{GP}(\varphi^{gs}) \rightarrow 0$ was shown in [72] for homogeneous gases. Here, Ψ^{gs} and φ^{gs} denote the (approximate) minimizers of the respective functionals. In case of a repulsive potential $V \geq 0$, the respective convergence was shown in [42]. In [43] it is shown that $\mu^{\Psi^{gs}} \rightarrow |\varphi^{gs}\rangle\langle\varphi^{gs}|$.

(b) Part (b) is a direct consequence of the estimate given in [60]. We restate a remark given in [60] about the uniform convergence in t :

By Sobolev's inequality, it follows that $\|\nabla\varphi_s\|_{6,loc} \leq \|\nabla\varphi_s\|_6 \leq \|\Delta\varphi\|$. Thus $\|\nabla\varphi_s\|_{6,loc}$ can be bounded controlling $\langle\varphi_s, (h^{GP})^2 \varphi_s\rangle$ sufficiently well.

On the other hand, $\|\nabla\varphi_s\|_{6,loc} \leq \|\nabla\varphi_s\|_\infty$. Since we are in the defocussing regime one expects, after the potential is turned off, that $\|\varphi\|_\infty$ and $\|\nabla\varphi\|_\infty$ decay like $t^{-3/2}$. Whenever this is the case $\int_0^\infty \|\varphi_s\|_\infty + \|\nabla\varphi_s\|_{6,loc} + \|\dot{A}_s\|_\infty ds < \infty$ and we get convergence uniformly in t .

- (c) The condition $\varphi_t \in H^2(\mathbb{R}^3, \mathbb{C})$ can be proven for a large class of external potentials, assuming sufficient regularity of the initial datum φ_0 , see e.g. [12].
- (d) The proof of Theorem 4.2.6 implies that the rate of convergence is of order $N^{-\delta}$ for some $\delta > 0$, assuming that $|\gamma_{\Psi_0}^{(1)} - |\varphi_0\rangle\langle\varphi_0|| \leq CN^{-2\delta}$, as well as assuming that the convergence rate of $\lim_{N \rightarrow \infty} \mathcal{E}(\Psi_0) = \mathcal{E}^{GP}(\varphi_0)$ to be least of order $N^{-2\delta}$.

4.3 Proof of Theorem 4.2.6

Notation 4.3.1 In the following, we will denote by $\mathcal{K}(\varphi_t, A_t)$ a constant, depending on $\|\varphi_t\|_{H^2(\mathbb{R}^3, \mathbb{C})}$ and on $\|A_t\|_\infty, \int_0^t ds \|\dot{A}_s\|_\infty$. Under the assumptions of Theorem 4.2.6, there exists a constant C_t , depending on t , such that $\mathcal{K}(\varphi_t, A_t) \leq C_t$.

In this chapter we will focus on the modifications one needs to perform in order to generalize the result of [60] to more general interactions V . Many Lemmata which were proven in [60] are valid for generic interaction potentials V and need not to be modified. We will therefore often omit parts of existing proofs and refer the reader to [60] for the detailed steps and motivations; see also Chapter 3 for the proof of the two dimensional case.

First, we will recall some important definitions we will need during the proof.

Definition 4.3.2 For any $1 \leq j \neq k \leq N$, let

$$a_{j,k} := \{(x_1, x_2, \dots, x_N) \in \mathbb{R}^{3N} : |x_j - x_k| < N^{-26/27}\}, \quad (4.16)$$

$$\overline{\mathcal{A}}_j := \bigcup_{k \neq j} a_{j,k} \quad \mathcal{A}_j := \mathbb{R}^{3N} \setminus \overline{\mathcal{A}}_j \quad \overline{\mathcal{B}}_j := \bigcup_{k,l \neq j} a_{k,l} \quad \mathcal{B}_j := \mathbb{R}^{3N} \setminus \overline{\mathcal{B}}_j. \quad (4.17)$$

In the following, we will state a general criteria under which assumptions on Ψ_t Theorem 4.2.6 is valid (see (b),(c) and (d) below). Subsequently, we prove that these assumptions are valid if the potential V fulfills Assumption 4.2.3.

Lemma 4.3.3 *Let $\Psi_0 \in L_s^2(\mathbb{R}^{3N}, \mathbb{C}) \cap H^2(\mathbb{R}^{3N}, \mathbb{C})$ with $\|\Psi_0\| = 1$. Let $\varphi_0 \in H^2(\mathbb{R}^3, \mathbb{C})$ with $\|\varphi_0\| = 1$. Let $\lim_{N \rightarrow \infty} \gamma_{\Psi_0}^{(1)} = |\varphi_0\rangle\langle\varphi_0|$ in trace norm as well as $\lim_{N \rightarrow \infty} \mathcal{E}(\Psi_0) = \mathcal{E}^{GP}(\varphi_0)$. Let Ψ_t the unique solution to $i\partial_t \Psi_t = H\Psi_t$ with initial datum Ψ_0 and assume $V \in L_c^\infty(\mathbb{R}^3, \mathbb{R})$ spherically symmetric. Let φ_t the unique solution to $i\partial_t \varphi_t = h^{GP} \varphi_t$ with initial datum φ_0 . Assume $A_t, \dot{A}_t \in L^\infty(\mathbb{R}^3, \mathbb{R})$. If,*

(a)

$$\varphi_t \in H^2(\mathbb{R}^3, \mathbb{C}). \quad (4.18)$$

(b)

$$\|V_1(x_1 - x_2)\Psi_t\| \leq CN^{1/2}. \quad (4.19)$$

(c)

$$\|\nabla_1 \Psi_t\| \leq C. \quad (4.20)$$

(d) for some $\eta > 0$, the following inequality holds:

$$\|\mathbb{1}_{\mathcal{A}_1} \nabla_1 q_1^{\varphi_t} \Psi_t\|^2 + \|\mathbb{1}_{\bar{\mathcal{B}}_1} \nabla_1 \Psi_t\|^2 \leq C \left(\langle \Psi_t, \widehat{n}^{\varphi_t} \Psi_t \rangle + N^{-\eta} \right) + |\mathcal{E}(\Psi_t) - \mathcal{E}^{GP}(\varphi_t)|. \quad (4.21)$$

(e)

$$V \text{ is chosen such that Lemma 4.3.8 is fulfilled.} \quad (4.22)$$

Then, for any $t > 0$

$$\lim_{N \rightarrow \infty} \gamma_{\Psi_t}^{(1)} = |\varphi_t\rangle\langle\varphi_t| \quad (4.23)$$

in trace norm.

Remark 4.3.4 *It has been shown in [60] that the Conditions (4.19), (4.20), (4.21) and (4.22) are fulfilled for nonnegative potentials $V \in L_c^\infty(\mathbb{R}^3, \mathbb{R})$. Conditions (4.19)-(4.21) are essentially those conditions which are non-trivial to prove and also lead to the class of potentials 4.2.3 we consider in this chapter.*

Proof: We like to recall the scheme of the proof of the equivalent of Theorem 4.2.6 for nonnegative potentials. As in Chapter 3, Definition 3.4.7, the functionals $\gamma_x(\Psi_t, \varphi_t)$, with $x \in \{a, b, c, d, e, f\}$ were used in [60] to obtain a Grönwall estimate¹. The exact definition of the functionals used for the three dimensional case can be found in Definition 6.2.

¹The functional called $\gamma_f(\Psi_t, \varphi_t)$ is actually missing in [60]. The definition of this functional can be found in equation (6.10) [49]. There, it is furthermore shown that the respective bound $|\gamma_f(\Psi_t, \varphi_t)| \leq \mathcal{K}(\varphi_t, A_t)N^{-\delta}$, $\delta > 0$ holds, assuming $V \in L_c^\infty(\mathbb{R}^3, \mathbb{R})$ to be nonnegative.

and Definition 6.3. in [60]. It is then proven in Lemma A.1. in [60] that the bound $|\gamma_x(\Psi_t, \varphi_t)| \leq \mathcal{K}(\varphi_t, A_t)(\alpha(\Psi_t, \varphi_t) + N^{-\delta})$, $x \in \{a, b, c, d, e\}$, $\delta > 0$ is valid for nonnegative potentials $V \in L_c^\infty(\mathbb{R}^3, \mathbb{C})$.

In the following, we will show that the estimates given in [60] remain valid under the Conditions (4.18)-(4.22). Note that we will not restate the estimates given in [60], but only focus on the modifications one needs to perform.

The bound of $\gamma_a(\Psi_t, \varphi_t)$ is the same as given in Lemma 3.5.6 and follows from $\dot{A}_t \in L^\infty(\mathbb{R}^3, \mathbb{R})$. The required bound for $\gamma_b(\Psi_t, \varphi_t)$ is derived in Lemma A.4., pp.31-37 in [60]. Following the estimates given in [60], it can be verified line-by-line that the given bounds are valid, if Conditions (4.18)-(4.22) and $A_t \in L^\infty(\mathbb{R}^3, \mathbb{R})$ hold. Furthermore, it can be verified that the functionals γ_c and γ_e can be controlled using Conditions (4.18)-(4.22), see Lemma A.1. and pp.38-42 in [60]. The estimate for γ_f is valid under Conditions (4.18) and (4.22) and can be found in p. 34 in [49].

The functional γ_d can be bounded, using the following estimate: Let $m^a(k) = m(k) - m(k+1)$, where, for some $\xi > 0$,

$$m(k) = \begin{cases} \sqrt{k/N}, & \text{for } k \geq N^{1-2\xi}, \\ 1/2(N^{-1+\xi}k + N^{-\xi}), & \text{else.} \end{cases}$$

We control

$$N^3 \left| \langle \Psi_t, \mathbb{1}_{\bar{\mathcal{B}}_1} g_{\beta_1,1}(x_1 - x_3) V_1(x_1 - x_2) \widehat{m^a}^{\varphi_t} p_1^{\varphi_t} \mathbb{1}_{\mathcal{B}_3} \Psi_t \rangle \right|, \quad (4.24)$$

where $g_{\beta_1,1}$ is defined in Lemma 4.3.8. This term, which appears in (A.49) in [60] is the only term in $\gamma_x(\Psi_t, \varphi_t)$, $x \in \{a, b, c, d, e, f\}$ where the estimates given in [60] needs to be modified, using only the assumptions given in the Lemma above. Using Lemma (2.0.10) with

$$\Omega = N^{-1/2} \mathbb{1}_{\mathcal{B}_3} V_1(x_1 - x_2) \Psi_t, \quad O_{1,2} = N^{7/2+\epsilon} g_{\beta_1,1}(x_1 - x_3) \mathbb{1}_{\bar{\mathcal{B}}_1} \widehat{m^a}^{\varphi_t} p_1^{\varphi_t} \mathbb{1}_{\mathcal{B}_3}, \quad \chi = \Psi_t$$

and $\epsilon > 0$ arbitrary, it then follows

$$(4.24) \leq N^{-1-\epsilon} \|\mathbb{1}_{\bar{\mathcal{B}}_1} V_1(x_1 - x_2) \Psi_t\|^2 \quad (4.25)$$

$$+ C N^{6+\epsilon} \|g_{\beta_1,1}(x_1 - x_3) \mathbb{1}_{V_1}(x_1 - x_2) \widehat{m^a}^{\varphi_t} p_1^{\varphi_t} \mathbb{1}_{\mathcal{B}_3} \Psi_t\|^2 \quad (4.26)$$

$$+ C N^{7+\epsilon} \left| \langle \Psi_t, \mathbb{1}_{\mathcal{B}_3} p_1^{\varphi_t} \widehat{m^a}^{\varphi_t} g_{\beta_1,1}(x_1 - x_3) \right. \\ \left. \times \mathbb{1}_{V_1}(x_1 - x_2) g_{\beta_1,1}(x_1 - x_4) \widehat{m^a}^{\varphi_t} p_1^{\varphi_t} \mathbb{1}_{\mathcal{B}_4} \Psi_t \rangle \right|. \quad (4.27)$$

For nonnegative V and $\epsilon = 0$, it was possible to control (4.25) using a specific energy estimate, see Lemma 5.2.(3) in [60]. We do not expect this estimate to hold for potentials V which are not nonnegative. For an interaction potential V , fulfilling Condition (4.19), we can however bound

$$(4.25) \leq C N^{-\epsilon}.$$

The estimate (4.26) $\leq \mathcal{K}(\varphi_t, A_t)N^{-1+2\xi+\epsilon}$ given in (A.51) [60] is valid under conditions (4.18)-(4.22). Note that Condition (4.22) implies $\|g_{\beta_1,1}(x_1 - x_2)\Omega\| \leq CN^{-1}\|\nabla_1\Omega\|$ for $\Omega \in L^2(\mathbb{R}^{3N}, \mathbb{C})$, see Lemma 4.3.8. This is one key estimate in order to bound (4.26). Under the same conditions, it has been shown (c.f. (A.52) in [60]) that

$$(4.27) \leq \mathcal{K}(\varphi_t, A_t)N^{-\frac{26}{9}+3\xi+\epsilon}.$$

Therefore, it follows for some $\eta > 0$ that

$$(4.24) \leq \mathcal{K}(\varphi_t, A_t)N^{-\eta} \quad (4.28)$$

holds by choosing $\xi > 0$ and $\epsilon > 0$ small enough².

□

Proof of Theorem 4.2.6: In the following, we will prove the Inequalities (4.19), (4.20) and (4.21) for interaction potentials which fulfill Assumption 4.2.3. Theorem 4.2.6, part (a) then follows from Lemma 4.3.3, together with the estimates given in Section 4.3.1. Part (b) of Theorem 4.2.6 follows from part (a) and the estimates given in [60].

□

4.3.1 The scattering state

In this section we analyze the microscopic structure which is induced by V_1 . While the principle estimates are the same as in [60], we need to modify the proofs given there which relied on the nonnegativity of V . The presentation is analogous to Chapter 3, Section 3.3, which is concerned with the scattering state in two dimensions.

Definition 4.3.5 *Let $V \in L_c^\infty(\mathbb{R}^3, \mathbb{R})$ fulfill Assumption 4.2.3. Define the zero energy scattering state j by*

$$\begin{cases} (-\Delta_x + \frac{1}{2}V(x))j(x) = 0, \\ \lim_{|x| \rightarrow \infty} j(x) = 1. \end{cases} \quad (4.29)$$

Furthermore define the scattering length a by

$$a = \text{scat}\left(\frac{1}{2}V\right) = \frac{1}{4\pi} \int \frac{1}{2}V(x)j(x)d^3x. \quad (4.30)$$

We want to recall some important properties of the scattering state j , see also Appendix C of [41].

² Note that the factors $N^{2\xi}$ and $N^{3\xi}$ are due to the definition of $m(k)$. A factor of the form $N^{s\xi}$, $s \in \{1, 2, 3\}$ also appears in the other functionals $\gamma_x(\Psi_t, \varphi_t)$, $x \in \{b, c, e, f\}$. It therefore follows that the the respective bounds $|\gamma_x(\Psi_t, \varphi_t)| \leq CN^{-\eta}$, $\eta > 0$ given in [60] are valid choosing $\xi > 0$ small enough. We like to remark that one cannot choose $\xi = 0$, since the convergence of the reduced density matrices stated in Lemma 4.3.3 does only follow for $0 < \xi < 1/2$, see [60] for the precise argument.

Lemma 4.3.6 *For the scattering state defined previously the following relations hold:*

(a) *j is a nonnegative, monotone nondecreasing function which is spherically symmetric in $|x|$. For $|x| \geq R$, j is given by*

$$j(x) = 1 - \frac{a}{|x|}.$$

(b) *The scattering length a fulfills $a \geq 0$.*

Proof:

(a)+(b) Since we assume $-\Delta + \frac{1}{2}V \geq 0$, one can define the scattering state j by a variational principle. Theorem C.1 in [41] then implies that j is a nonnegative, spherically symmetric function in $|x|$ such that $j(x) = 1 - \frac{a}{|x|}$ holds for $|x| \geq R$ with $a \in \mathbb{R}$ defined as in Eq. (4.30). By Condition (4.10) it follows $a \geq 0$, see Theorem C.1., (C.8.) in [41]. It is only left to show that j is monotone nondecreasing in $|x|$. Let $t(|x|) = j(x)$ and define

$$a_r = \frac{1}{4\pi} \int_0^r \frac{1}{2}V(r'e_{r'})t(r')(r')^2 dr',$$

where $e_{r'}$ denotes the radial unit vector. Note that $a = \lim_{r \rightarrow \infty} a_r = a_R$. By Gauß-theorem and the scattering equation (4.29), it then follows for $r > 0$

$$\frac{d}{dr}t(r) = \frac{a_r}{r^2}.$$

Since $t(r) \geq 0$ holds for all $r \geq 0$, it follows $a_r > 0$ for all $r \in]0, r_2[$. If it were now that j is not monotone nondecreasing, there must exist a $\tilde{r} \geq r_2$, such that $a_{\tilde{r}} < 0$. $V(x) \leq 0$ and $t(r) \geq 0$ for all $|x| \in]r_2, R[$ then imply $a_r \leq a_{\tilde{r}}$ for all $r \geq \tilde{r}$. This, however, contradicts $a = a_R \geq 0$. Thus, it follows that j is monotone nondecreasing.

□

As in Chapter 3, Section 3.3, we will define a potential W_{β_1} with $0 < \beta_1 < 1$, such that $\frac{1}{2}(V_1 - W_{\beta_1})$ has scattering length zero. This allows us to “replace” V_1 by W_{β_1} , which has better scaling behavior and is easier to control.

Definition 4.3.7 *Let $V \in L_c^\infty(\mathbb{R}^3, \mathbb{R})$ satisfy Assumption 4.2.3. For any $0 < \beta_1 < 1$ and any $R_{\beta_1} \geq N^{-\beta_1}$ we define the potential W_{β_1} via*

$$W_{\beta_1}(x) = \begin{cases} aN^{3\beta_1-1} & \text{if } N^{-\beta_1} < |x| \leq R_{\beta_1}, \\ 0 & \text{else.} \end{cases} \quad (4.31)$$

Furthermore, we define the zero energy scattering state $f_{\beta_1,1}$ of the potential $\frac{1}{2}(V_1 - W_{\beta_1})$, that is

$$\begin{cases} \left(-\Delta_x + \frac{1}{2}(V_1(x) - W_{\beta_1}(x)) \right) f_{\beta_1,1}(x) = 0, \\ f_{\beta_1,1}(x) = 1 \text{ for } |x| = R_{\beta_1}. \end{cases} \quad (4.32)$$

In the following Lemma we show that there exists a minimal value R_{β_1} such that the scattering length of the potential $\frac{1}{2}(V_1 - W_{\beta_1})$ is zero.

Lemma 4.3.8 *For the scattering state $f_{\beta_1,1}$, defined by (4.32), the following relations hold:*

(a) *There exists a minimal value $R_{\beta_1} \in \mathbb{R}$ such that $\int(V_1(x) - W_{\beta_1}(x))f_{\beta_1,1}(x)d^3x = 0$.*

For the rest of this chapter we assume that R_{β_1} is chosen such that (a) holds.

(b) *There exists $K_{\beta_1} \in \mathbb{R}$, $K_{\beta_1} > 0$ such that $K_{\beta_1}f_{\beta_1,1}(x) = j(Nx) \forall |x| \leq N^{-\beta_1}$.*

(c) *$f_{\beta_1,1}$ is a nonnegative, monotone nondecreasing function in $|x|$. Furthermore,*

$$f_{\beta_1,1}(x) = 1 \text{ for } |x| \geq R_{\beta_1}. \quad (4.33)$$

(d)

$$1 \geq K_{\beta_1} \geq 1 - \frac{a}{N^{1-\beta_1}}. \quad (4.34)$$

(e) $R_{\beta_1} \leq CN^{-\beta_1}$.

For any fixed $0 < \beta_1$, N sufficiently large such that V_1 and W_{β_1} do not overlap, we obtain

(f)

$$|N\|V_1f_{\beta_1,1}\|_1 - 8\pi a| = |N\|W_{\beta_1}f_{\beta_1,1}\|_1 - 8\pi a| \leq CN^{-1-\beta_1}.$$

(g) *Define*

$$g_{\beta_1,1}(x) = 1 - f_{\beta_1,1}(x).$$

Then,

$$\|g_{\beta_1,1}\|_1 \leq CN^{-1-2\beta_1}, \|g_{\beta_1,1}\|_{3/2} \leq CN^{-1-\beta_1}, \|g_{\beta_1,1}\| \leq CN^{-1-\beta_1/2}, \|g_{\beta_1,1}\|_\infty \leq 1.$$

(h)

$$|N\|W_{\beta_1}\|_1 - 8\pi a| \leq CN^{-1+\beta_1}.$$

(i) *For any $\Omega \in H^1(\mathbb{R}^{3N}, \mathbb{C})$, we have*

$$\|g_{\beta_1,1}(x_1 - x_2)\Omega\| \leq CN^{-1}\|\nabla_1\Omega\|.$$

Proof:

4. Derivation of the Gross-Pitaevskii Equation for a Class of Non Purely Positive Potentials

(a) In the following, we will sometimes denote, with a slight abuse of notation, $f_{\beta_1,1}(x) = f_{\beta_1,1}(r)$ and $j(x) = j(r)$ for $r = |x|$ (for this, recall that $f_{\beta_1,1}$ and j are radially symmetric). We further denote by $f'_{\beta_1,1}(r)$ the derivative of $f_{\beta_1,1}$ with respect to the radial coordinate r . We first show by contradiction that $f_{\beta_1,1}(N^{-\beta_1}) \neq 0$. For this, assume that $f_{\beta_1,1}(x) = 0$ for all $|x| \leq N^{-\beta_1}$. Since $f_{\beta_1,1}$ is continuous, there exists a maximal value $r_0 \geq N^{-\beta_1}$ such that the scattering equation (4.32) is equivalent to

$$\begin{cases} \left(-\Delta_x - \frac{1}{2}W_{\beta_1}(x) \right) f_{\beta_1,1}(x) = 0, \\ f_{\beta_1,1}(x) = 1 \text{ for } |x| = R_{\beta_1}, \\ f_{\beta_1,1}(x) = 0 \text{ for } |x| \leq r_0. \end{cases} \quad (4.35)$$

Using (4.32) and Gauss'-theorem, we further obtain

$$f'_{\beta_1,1}(r) = \frac{1}{8\pi r^2} \int_{B_r(0)} d^3x (V_1(x) - W_{\beta_1}(x)) f_{\beta_1,1}(x). \quad (4.36)$$

(4.35) and (4.36) then imply for $r > r_0$

$$\begin{aligned} |f'_{\beta_1,1}(r)| &= \frac{1}{8\pi r^2} \left| \int_{B_r(0)} d^3x W_{\beta_1}(x) f_{\beta_1,1}(x) \right| = \frac{aN^{-1+3\beta_1}}{2r^2} \left| \int_{r_0}^r dr' r'^2 f_{\beta_1,1}(r') \right| \\ &\leq \frac{aN^{-1+3\beta_1}}{2r^2} \left| \int_{r_0}^r dr' r'^2 (r' - r_0) \sup_{r_0 \leq s \leq r} |f'_{\beta_1,1}(s)| \right|. \end{aligned}$$

Taking the supreme over the interval $[r_0, r]$, the inequality above then implies that there exists a constant $C(r, r_0) \neq 0$, $\lim_{r \rightarrow r_0} C(r, r_0) = 0$ such that $\sup_{r_0 \leq s \leq r} |f'_{\beta_1,1}(s)| \leq C(r, r_0) N^{-1+3\beta_1} \sup_{r_0 \leq s \leq r} |f'_{\beta_1,1}(s)|$. Thus, for r close enough to r_0 , the inequality above can only hold if $f'_{\beta_1,1}(s) = 0$ for $s \in [r_0, r]$, yielding a contradiction to the choice of r_0 .

Consequently, there exists a $x_0 \in \mathbb{R}^3$, $|x_0| \leq N^{-\beta_1}$, such that $f_{\beta_1,1}(x_0) \neq 0$. We can thus define

$$h(x) = f_{\beta_1,1}(x) \frac{j(Nx_0)}{f_{\beta_1,1}(x_0)}$$

on the compact set $\overline{B_{x_0}(0)}$. One easily sees that $h(x) = \frac{j(Nx)}{f_{\beta_1,1}(x_0)}$ on $\partial \overline{B_{x_0}(0)}$ and satisfies the zero energy scattering equation (4.29) for $x \in \overline{B_{N^{-\beta_1}}(0)}$. Note that the scattering equations (4.29) and (4.32) have a unique solution on any compact set. It then follows that $h(x) = j(Nx) \forall x \in \overline{B_{N^{-\beta_1}}(0)}$. Since $j(NN^{-\beta_1}) \neq 0$, we then obtain $f_{\beta_1,1}(N^{-\beta_1}) \neq 0$.

Thus, $f_{\beta_1,1}(x) = j(Nx) \frac{f_{\beta_1,1}(x_0)}{j(Nx_0)}$ holds for all $|x| \leq N^{-\beta_1}$ and for all $x_0 \in]0, N^{-\beta_1}]$. Lemma 4.3.6 further implies that either $f_{\beta_1,1}$ or $-f_{\beta_1,1}$ is a nonnegative, spherically symmetric and monotone nondecreasing function in $|x|$ for all $|x| \leq N^{-\beta_1}$.

Recall that W_{β_1} and hence $f_{\beta_1,1}(x)$ depend on $R_{\beta_1} \in [N^{-\beta_1}, \infty[$. For conceptual clarity, we denote $W_{\beta_1}^{(R_{\beta_1})}(x) = W_{\beta_1}(x)$ and $f_{\beta_1,1}^{(R_{\beta_1})}(x) = f_{\beta_1,1}(x)$ for the rest of the proof of part (a). For β_1 fixed, consider the function

$$s : [N^{-\beta_1}, \infty[\rightarrow \mathbb{R} \quad (4.37)$$

$$R_{\beta_1} \mapsto \int_{B_{R_{\beta_1}}(0)} d^3x (V_1(x) - W_{\beta_1}^{(R_{\beta_1})}(x)) f_{\beta_1,1}^{(R_{\beta_1})}(x). \quad (4.38)$$

We show by contradiction that the function s has at least one zero. Assume $s \neq 0$ were to hold. We can assume w.l.o.g. $s > 0$. It then follows from Gauss'-theorem that $f_{\beta_1,1}^{(R_{\beta_1})}(R_{\beta_1}) > 0$ for all $R_{\beta} \geq N^{-\beta_1}$. By uniqueness of the solution of the scattering equation (4.32), for $\tilde{R}_{\beta_1} < R_{\beta_1}$ there exists a constant $K_{\tilde{R}_{\beta_1}, R_{\beta_1}} \neq 0$, such that for all $|x| \leq \tilde{R}_{\beta_1}$ we have $f_{\beta_1,1}^{(\tilde{R}_{\beta_1})}(x) = K_{\tilde{R}_{\beta_1}, R_{\beta_1}} f_{\beta_1,1}^{(R_{\beta_1})}(x)$. If $K_{\tilde{R}_{\beta_1}, R_{\beta_1}} < 0$ were to hold, we could conclude from

$$0 < s(\tilde{R}_{\beta_1}) = 8\pi(\tilde{R}_{\beta_1})^2 f_{\beta_1,1}^{(\tilde{R}_{\beta_1})}(\tilde{R}_{\beta_1}) = 8\pi(\tilde{R}_{\beta_1})^2 K_{\tilde{R}_{\beta_1}, R_{\beta_1}} f_{\beta_1,1}^{(R_{\beta_1})}(\tilde{R}_{\beta_1})$$

that $f_{\beta_1,1}^{(R_{\beta_1})}(\tilde{R}_{\beta_1}) < 0$. By continuity of $f_{\beta_1,1}^{(R_{\beta_1})}$ and $f_{\beta_1,1}^{(R_{\beta_1})}(R_{\beta_1}) > 0$, there exists $r \in]\tilde{R}_{\beta_1}, R_{\beta_1}[$, such that $0 = f_{\beta_1,1}^{(R_{\beta_1})}(r) = K_{R_{\beta_1}, r} f_{\beta_1,1}^{(r)}(r)$, yielding to a contradiction to $s > 0$.

We can therefore conclude $K_{\tilde{R}_{\beta_1}, R_{\beta_1}} > 0$. From Lemma 4.3.6, the assumption $s(N^{-\beta_1}) > 0$ and $K_{\tilde{R}_{\beta_1}, R_{\beta_1}} > 0$, we obtain, for all $r \in [0, N^{-\beta_1}]$ and for all $R_{\beta_1} \in [N^{-\beta_1}, \infty[$, that $f_{\beta_1,1}^{(R_{\beta_1})}(r) \geq 0$ holds. From $s \neq 0$, it then follows that, for all $r \in [N^{-\beta_1}, \infty[$ and for all $R_{\beta_1} \in [N^{-\beta_1}, \infty[$, $f_{\beta_1,1}^{(R_{\beta_1})}(r) \neq 0$. Thus, for all $r \in [N^{-\beta_1}, \infty[$ and for all $R_{\beta_1} \in [N^{-\beta_1}, \infty[$, the function $f_{\beta_1,1}^{(R_{\beta_1})}(r)$ doesn't change sign. This, however, implies $\lim_{R_{\beta_1} \rightarrow \infty} s(R_{\beta_1}) = -\infty$ yielding to a contradiction. By continuity of s , there exists thus a minimal value $R_{\beta_1} \geq N^{-\beta_1}$ such that $s(R_{\beta_1}) = 0$.

Remark 4.3.9 As mentioned, we will from now on fix $R_{\beta_1} \in [N^{-\beta_1}, \infty[$ as the minimal value such that $s(R_{\beta_1}) = 0$. Furthermore, we may assume $a > 0$ and $R_{\beta_1} > N^{-\beta_1}$ in the following. For $a = 0$, we can choose $R_{\beta_1} = N^{-\beta_1}$, such that $f_{\beta_1,1}(x) = j(Nx)/j(NN^{-\beta_1})$. It is then easy to verify that the Lemma stated is valid.

(b) From $j(Nx) = f_{\beta_1,1}(x) \frac{j(NN^{-\beta_1})}{f_{\beta_1,1}(N^{-\beta_1})}$, for all $|x| \leq N^{-\beta_1}$, we can conclude that

$$K_{\beta_1} = \frac{j(NN^{-\beta_1})}{f_{\beta_1,1}(N^{-\beta_1})}. \quad (4.39)$$

Next, we show that the constant K_{β_1} is positive. Since $j(NN^{-\beta_1})$ is positive, it follows from Eq. (4.39) that K_{β_1} and $f_{\beta_1,1}(N^{-\beta_1})$ have equal sign. By (a), the sign of

$f_{\beta_1,1}$ is constant for $|x| \leq R_{\beta_1}$. Furthermore, from Gauss' theorem and the scattering equation (4.32) we have

$$f'_{\beta_1,1}(r) = \frac{1}{8\pi r^2 K_{\beta_1}} \int_{B_r(0)} V_1(x) j(Nx) d^3x \quad (4.40)$$

for all $0 < r \leq N^{-\beta_1}$. Since $\int_{B_r(0)} V_1(x) j(Nx) d^3x$ is nonnegative for all $0 < r \leq N^{-\beta_1}$ (see the proof of Lemma 4.3.6), we then conclude

$$\operatorname{sgn}(f'_{\beta_1,1}(N^{-\beta_1})) = \operatorname{sgn}(K_{\beta_1}). \quad (4.41)$$

Recall that $f'_{\beta_1,1}(R_{\beta}) = 0$. If it were now that K_{β_1} is negative, we could conclude from (4.39) and (4.41) that $f'_{\beta_1,1}(N^{-\beta_1}) < 0$ and $f_{\beta_1,1}(N^{-\beta_1}) < 0$. Since R_{β_1} is by definition the smallest value where $f'_{\beta_1,1}$ vanishes, we were able to conclude from the continuity of the derivative that $f'_{\beta_1,1}(r) < 0$ for all $r < R_{\beta_1}$ and hence $f(R_{\beta_1}) < 0$. However, this were in contradiction to the boundary condition of the zero energy scattering state (see (4.32)) and thus $K_{\beta_1} > 0$ follows.

- (c) From the proof of property (b), we see that $f_{\beta_1,1}$ and its derivative is positive at $N^{-\beta_1}$. From (4.36), we obtain $f'_{\beta_1,1}(r) = 0$ for all $r > R_{\beta_1}$. Thus $f_{\beta_1,1}(x) = 1$ for all $|x| \geq R_{\beta_1}$. Due to continuity $f'_{\beta_1,1}(r) > 0$ for all $r < R_{\beta_1}$. Since $f_{\beta_1,1}$ is continuous, positive at $N^{-\beta_1}$, and its derivative is a nonnegative function, it follows that $f_{\beta_1,1}$ is a nonnegative, monotone nondecreasing function in $|x|$.
- (d) Since $f_{\beta_1,1}$ is a positive monotone nondecreasing function in $|x|$, we obtain

$$1 \geq f_{\beta_1,1}(N^{-\beta_1}) = j(NN^{-\beta_1})/K_{\beta_1} = \left(1 - \frac{a}{N^{1-\beta_1}}\right)/K_{\beta_1}.$$

We obtain the lower bound

$$K_{\beta_1} \geq 1 - \frac{a}{N^{1-\beta_1}}.$$

For the upper bound, we first prove that $f_{\beta}(x) \geq j(Nx)/j(NR_{\beta_1})$ holds for all $|x| \leq N^{-\beta_1}$. Define $m(x) = j(Nx)/j(NR_{\beta_1}) - f_{\beta_1,1}(x)$. Using the scattering equations (4.29) and (4.32), we obtain

$$\begin{cases} \Delta_x m(x) = \frac{1}{2}V_1(x)m(x) + \frac{1}{2}W_{\beta_1}(x)f_{\beta_1,1}(x), \\ m(R_{\beta_1}) = 0. \end{cases} \quad (4.42)$$

Since $W_{\beta_1}(x)f_{\beta_1,1}(x) \geq 0$, we obtain that $\Delta_x m(x) \geq 0$ for $N^{-1}R \leq |x| \leq R_{\beta_1}$. That is, $m(x)$ is subharmonic for $N^{-1}R < |x| < R_{\beta_1}$. Using the maximum principle, we obtain, using that $m(x)$ is spherically symmetric

$$\max_{N^{-1}R \leq |x| \leq R_{\beta_1}} (m(x)) = \max_{|x| \in \{N^{-1}R, R_{\beta_1}\}} (m(x)). \quad (4.43)$$

If it were now that $\max_{|x| \in \{N^{-1}R, R_{\beta_1}\}}(m(x)) = m(N^{-1}R) \geq m(R_{\beta}) = 0$, we could assume $m(x) > 0$ for all $N^{-1}R \leq |x| \leq N^{-\beta_1}$ (otherwise we would have $m(N^{-\beta_1}) = 0$, which implies $K_{\beta_1} = j(NR_{\beta_1}) = 1 - \frac{a}{NR_{\beta_1}} \leq 1$). Note that $m(x)$ then solves

$$\begin{cases} -\Delta_x m(x) + \frac{1}{2}V_1(x)m(x) = 0 & \text{for } |x| \leq N^{-\beta_1}, \\ m(N^{-1}R) > 0. \end{cases}$$

By Theorem C.1 in [41] (note that we can assume $a > 0$), m is strictly increasing for $N^{-1}R \leq |x| \leq N^{-\beta_1}$. This, however, contradicts $\max_{|x| \in \{N^{-1}R, R_{\beta_1}\}}(m(x)) = m(N^{-1}R)$.

Therefore, we can conclude in (4.43) that $\max_{|x| \in \{N^{-1}R, R_{\beta_1}\}}(m(x)) = m(R_{\beta_1}) = 0$ holds. Then, it follows that $f_{\beta}(x) - j(Nx)/j(NR_{\beta_1}) \geq 0$ for all $N^{-1}R \leq |x| \leq N^{-\beta_1}$. Using the zero energy scattering equation

$$-\Delta(f_{\beta_1,1}(x) - j(Nx)/j(NR_{\beta_1})) + \frac{1}{2}V_1(x)(f_{\beta_1,1}(x) - j(Nx)/j(NR_{\beta_1})) = 0$$

for $|x| \leq N^{-\beta_1}$, we can, together with $f_{\beta_1,1}(N^{-\beta_1}) - j(NN^{-\beta_1})/j(NR_{\beta_1}) \geq 0$, conclude that $f_{\beta_1,1}(x) - j(Nx)/j(NR_{\beta_1}) \geq 0$ for all $|x| \leq R_{\beta_1}$.

As a consequence, we obtain the desired bound $K_{\beta} = \frac{j(NN^{-\beta_1})}{f_{\beta_1,1}(N^{-\beta_1})} \leq j(NR_{\beta_1}) \leq 1$.

(e) Since $f_{\beta_1,1}$ is a nonnegative, monotone nondecreasing function in $|x|$, it follows that

$$\begin{aligned} N^{-1}f_{\beta_1,1}(N^{-\beta_1}) \int V(x)d^3x &= f_{\beta_1,1}(N^{-\beta_1}) \int V_1(x)d^3x \geq \int V_1(x)f_{\beta_1,1}(x)d^3x \\ &= \int W_{\beta_1}(x)f_{\beta_1,1}(x)d^3x \geq f_{\beta_1,1}(N^{-\beta_1}) \int W_{\beta_1}(x)d^3x. \end{aligned}$$

Therefore, $\int W_{\beta_1}(x)d^3x \leq CN^{-1}$ holds, which implies that $R_{\beta_1} \leq CN^{-\beta_1}$.

(f) Using

$$\|W_{\beta_1}f_{\beta_1,1}\|_1 = \|V_1f_{\beta_1,1}\|_1 = K_{\beta_1}^{-1}\|V_1j(N\cdot)\|_1 = K_{\beta_1}^{-1}8\pi\frac{a}{N},$$

we obtain

$$|N\|V_1f_{\beta_1,1}\|_1 - 8\pi a| = |N\|W_{\beta_1}f_{\beta_1,1}\|_1 - 8\pi a| = 8\pi|K_{\beta_1}^{-1} - 1| \leq CN^{-1+\beta_1}.$$

(g) Using for $|x| \leq R_{\beta_1}$ the inequality $1 \geq f_{\beta_1,1}(x) \geq j(Nx)/j(NR_{\beta_1})$, it follows for $|x| \leq R_{\beta_1}$

$$0 \leq g_{\beta_1,1}(x) = 1 - f_{\beta_1,1}(x) \leq 1 - j(Nx)/j(NR_{\beta_1}).$$

Let \tilde{j} solve

$$\begin{cases} \left(-\Delta_x + \frac{1}{2}V(x)\mathbb{1}_{|x| \leq r_2} \right) \tilde{j}(x) = 0, \\ \tilde{j}(2R) = j(2R). \end{cases}$$

It then follows that $\tilde{a} = \text{scat}\left(\frac{1}{2}V(x)\mathbb{1}_{|x| \leq r_2}\right) > 0$. Furthermore, it follows from Theorem C.1 and Lemma C.2 in [41] that

$$\tilde{j}(x) \geq \frac{1 - \frac{\tilde{a}}{|x|}}{1 - \frac{\tilde{a}}{2R}} j(2R) = \left(1 - \frac{\tilde{a}}{|x|}\right) \frac{1 - \frac{a}{2R}}{1 - \frac{\tilde{a}}{2R}}$$

holds for all $x \in \mathbb{R}^3$. Consider $n(x) = \tilde{j}(x) - j(x)$. n then solves

$$\begin{cases} \Delta_x n(x) = \frac{1}{2}V(x)n(x) + \frac{1}{2}V(x)\mathbb{1}_{|x| \leq r_2}\tilde{j}(x), \\ n(2R) = 0. \end{cases}$$

As before (see (4.42)), we can conclude $n(x) \leq 0$ for all $|x| \leq 2R$, which implies $j(x) \geq \tilde{j}(x)$, for $|x| \leq 2R$. Therefore,

$$j(Nx) \geq \begin{cases} \left(1 - \frac{\tilde{a}}{N|x|}\right)^{\frac{1-\frac{a}{2NR}}{1-\frac{\tilde{a}}{2NR}}} & \text{for } N|x| \leq R, \\ 1 - \frac{a}{N|x|} & \text{else.} \end{cases}$$

This implies, using part (d),

$$\begin{aligned} g_{\beta_1,1}(x) &\leq 1 - \begin{cases} \left(1 - \frac{\tilde{a}}{N|x|}\right)^{\frac{1-\frac{a}{2NR}}{(1-\frac{\tilde{a}}{2NR})(1-\frac{a}{NR\beta_1})}} & \text{for } N|x| \leq R, \\ \frac{1-\frac{a}{N|x|}}{(1-\frac{a}{NR\beta_1})} & \text{else.} \end{cases} \\ &\leq \begin{cases} \frac{\tilde{a}}{N|x|} + CN^{-1} & \text{for } N|x| \leq R, \\ \frac{a}{N|x|} + CN^{-1+\beta_1} & \text{else.} \end{cases} \end{aligned} \tag{4.44}$$

Since $g_{\beta_1,1}(x) = 0$ for $|x| > R_\beta$, we conclude with $R_{\beta_1} \leq CN^{-\beta_1}$ that

$$\|g_{\beta_1,1}\|_1 \leq N^{-1-2\beta_1},$$

as well as

$$\|g_{\beta_1,1}\|_{3/2} \leq CN^{-1-\beta_1}, \quad \|g_{\beta_1,1}\| \leq CN^{-1-\beta_1/2}.$$

Furthermore, $\|g_{\beta_1,1}\|_\infty = \|1 - f_{\beta_1,1}\|_\infty \leq 1$, since $f_{\beta_1,1}$ is a nonnegative, monotone nondecreasing function with $f_{\beta_1,1}(x) \leq 1$.

(h) Using (f) and (g), we obtain with $\|W_{\beta_1}\|_1 \leq CN^{-1}$

$$\begin{aligned} |N\|W_{\beta_1}\|_1 - 8\pi a| &\leq |N\|W_{\beta_1}f_{\beta_1,1}\|_1 - 8\pi a| + N\|W_{\beta_1}g_{\beta_1,1}\|_1 \\ &\leq C(N^{-1+\beta_1} + \|\mathbb{1}_{|\cdot| \geq N^{-\beta_1}}g_{\beta_1,1}\|_\infty). \end{aligned}$$

Since $g_{\beta_1,1}(x)$ is a nonnegative, monotone nonincreasing function, it follows with $K_{\beta_1} \leq 1$

$$\|\mathbb{1}_{|\cdot| \geq N^{-\beta_1}}g_{\beta_1,1}\|_\infty = g_{\beta_1,1}(N^{-\beta_1}) = 1 - f_{\beta_1,1}(N^{-\beta_1}) = 1 - \frac{j(NN^{-\beta_1})}{K_{\beta_1}} \leq aN^{-1+\beta_1}.$$

and (h) follows.

(i) Using the pointwise estimate (4.44), we obtain for any $\Omega \in H^1(\mathbb{R}^{3N}, \mathbb{C})$

$$\|g_{\beta_1,1}(x_1 - x_2)\Omega\| \leq C(N^{-1+\beta_1}\|\mathbb{1}_{B_{CN^{-\beta_1}}(0)}(x_1 - x_2)\Omega\| + N^{-1}\||x_1 - x_2|^{-1}\Omega\|).$$

Since $\||x_1 - x_2|^{-1}\Omega\| \leq 2\|\nabla_1\Omega\|$ as well as $\|\mathbb{1}_{B_{CN^{-\beta_1}}(0)}(x_1 - x_2)\Omega\| \leq CN^{-3\beta_1/2}\|\nabla_1\Omega\|$ holds, we obtain part (i).

□

4.3.2 Nonnegativity of the Hamiltonian

Next, we prove several important operator inequalities related to the Hamiltonian H , see Corollary 4.3.15. These inequalities will be used in order to show the Inequalities (4.19), (4.20) and (4.21).

Lemma 4.3.10 *Let $d \in \{2, 3\}$ and let $U \in L_c^\infty(\mathbb{R}^d, \mathbb{R})$ fulfill Assumption 4.2.3 and define*

$$H_U = -\sum_{k=1}^N \Delta_k + \sum_{i < j=1}^N U(x_i - x_j).$$

Then

$$H_U \geq 0.$$

In order to prove this Lemma, we first define

Definition 4.3.11 *Let $d \in \{2, 3\}$. For $\tilde{R} \geq 2R$, where R is defined as in Assumption 4.2.3, let for any $j, k = 1, \dots, N$ with $j \neq k$*

$$b_{j,k} := \{(x_1, x_2, \dots, x_N) \in \mathbb{R}^{dN} : |x_j - x_k| \leq \tilde{R}\}, \quad (4.45)$$

$$\bar{\mathcal{C}}_l := \bigcup_{j,k \neq l} b_{j,k}, \quad \mathcal{C}_l := \mathbb{R}^{dN} \setminus \bar{\mathcal{C}}_l.$$

Proof: Let

$$H_{\bar{\mathcal{C}}} = \sum_{k=1}^N -\Delta_k \mathbb{1}_{\bar{\mathcal{C}}_k} + \sum_{i \neq j} \mathbb{1}_{\bar{\mathcal{C}}_j} \frac{1}{2} U(x_i - x_j),$$

$$H_{\mathcal{C}} = \sum_{k=1}^N -\Delta_k \mathbb{1}_{\mathcal{C}_k} + \sum_{i \neq j} \mathbb{1}_{\mathcal{C}_j} \frac{1}{2} U(x_i - x_j).$$

Note that

$$H_{\mathcal{C}} = \sum_{k=1}^N -\Delta_k \mathbb{1}_{\mathcal{C}_k} + \frac{1}{4} \sum_{i \neq j} (\mathbb{1}_{\mathcal{C}_j} + \mathbb{1}_{\mathcal{C}_i}) \frac{1}{2} U(x_i - x_j)$$

is a symmetric operator w.r.t. to exchange of coordinates x_1, \dots, x_N . Therefore, it suffices to prove $\langle\langle \Psi, H_{\mathcal{C}} \Psi \rangle\rangle \geq 0$ for $\Psi \in L_s^2(\mathbb{R}^{dN}, \mathbb{C})$, since we can apply Theorem 3.3 and Corollary 3.1 in [40] to conclude

$$\inf_{\Psi \in L^2(\mathbb{R}^{dN}, \mathbb{C}), \|\Psi\|=1} \langle\langle \Psi, H_{\mathcal{C}} \Psi \rangle\rangle = \inf_{\Psi \in L_s^2(\mathbb{R}^{dN}, \mathbb{C}), \|\Psi\|=1} \langle\langle \Psi, H_{\mathcal{C}} \Psi \rangle\rangle.$$

In order to prove $H_{\mathcal{C}} \geq 0$, we show $K_1 = -\Delta_1 \mathbb{1}_{\mathcal{C}_1} + \frac{1}{2} \sum_{j=2}^N \mathbb{1}_{\mathcal{C}_1} \frac{1}{2} U(x_1 - x_j) \geq 0$ on $L_s^2(\mathbb{R}^{dN}, \mathbb{C})$. Since

$$\begin{aligned} \inf_{\Psi \in L_s^2(\mathbb{R}^{dN}, \mathbb{C}), \|\Psi\|=1} \langle\langle \Psi, H_{\mathcal{C}} \Psi \rangle\rangle &= \inf_{\Psi \in L_s^2(\mathbb{R}^{dN}, \mathbb{C}), \|\Psi\|=1} \sum_{i=1}^N \langle\langle \Psi, K_i \Psi \rangle\rangle \\ &= N \inf_{\Psi \in L_s^2(\mathbb{R}^{dN}, \mathbb{C}), \|\Psi\|=1} \langle\langle \Psi, K_1 \Psi \rangle\rangle \end{aligned}$$

holds, it then follows $H_{\mathcal{C}} \geq 0$.

The next Lemmata prove that $K_1 \geq 0$ and $H_{\bar{\mathcal{C}}} \geq 0$. Since $H_U = \sum_{i=1}^N K_i + H_{\bar{\mathcal{C}}}$, it then follows $H_U \geq 0$.

□

Remark 4.3.12 *The reason to split the Hamiltonian as done above is the following: The interaction $\mathbb{1}_{\bar{\mathcal{C}}_j} \frac{1}{2} U(x_i - x_j)$ is only nonzero, if, for fixed configurations (x_1, \dots, x_N) , x_i is closer than R to x_j , but no other particles are closer than R to neither x_i nor x_j . Therefore, the set $\bar{\mathcal{C}}$ excludes those configurations, where three-particle interactions occur. The strategy to separate the configurations of possible three-particle interactions is well known within the literature, see e.g. [41, 72] and references therein.*

Lemma 4.3.13 *Let K_1 and $H_{\bar{\mathcal{C}}}$ be defined as above. Under the assumptions of Lemma 4.3.10, we have*

(a)

$$K_1 \geq 0 \text{ on } L_s^2(\mathbb{R}^{dN}, \mathbb{C}).$$

(b)

$$H_{\bar{\mathcal{C}}} \geq 0 \text{ on } L^2(\mathbb{R}^{dN}, \mathbb{C}).$$

Proof:

- (a) The proof of Lemma 3.5.11, part (b) can be applied to prove part (a) in the case $d = 2$. Note for the proof to be valid, it is important that $\mathbb{1}_{\mathcal{C}_k}(x_1, \dots, x_N)$ excludes those configurations where the distance of two distinct particles x_i and x_j , $i, j \neq k$ to x_k is smaller than R , which is the radius of the support of U . For $d = 3$, it is easy to verify that the analogous proof of Lemma 3.5.11, as stated in Lemma 5.1. (3) in [60], can be applied.
- (b) **Remark 4.3.14** *The proof of part (b) originates from Lemma 10. in [72]. The author, however, does not introduce the set \mathcal{C}_k , but uses a different technique to exclude three particle interactions. For conceptual clarity, we adapt the proof of Lemma 10. in [72] to our definition of $H_{\bar{\mathcal{C}}}$. Since the proof given by Jun Yin is very elegant in our opinion, parts of the following proof are taken verbatim from [72].*

Recall that

$$H_{\bar{\mathcal{C}}} = \sum_{k=1}^N -\Delta_k \mathbb{1}_{\bar{\mathcal{C}}_k} + \sum_{i \neq j} \mathbb{1}_{\bar{\mathcal{C}}_j} \frac{1}{2} U(x_i - x_j).$$

Assume first that N is even, i.e., $N = 2N_1$ with $N_1 \in \mathbb{N}$. Let $P = (\pi_1, \pi_2)$ be a partition of $1, \dots, N$ into two disjoint sets with N_1 integers in π_1 and π_2 , respectively. Let

$$U_{1,1} = U_{2,2} = U^+ \geq 0, \quad U_{1,2} = 2U_1^+ - 4U^-, \quad (4.46)$$

with $U_{1,2}^- = -4U^-$, $U_{1,2}^+ = 2U^+$. It then follows

$$\frac{1}{4} (U_{1,1} + U_{2,1} + U_{2,2}) = U.$$

For each P , we define (for shorter notation, we will assume $i \neq j$ in the following)

$$\begin{aligned} H_P = H_{(\pi_1, \pi_2)} \equiv & \sum_{j \in \pi_1} -2\Delta_j \mathbb{1}_{\bar{\mathcal{C}}_j} + \sum_{i,j \in \pi_1} \mathbb{1}_{\bar{\mathcal{C}}_j} \frac{1}{2} U_{1,1}(x_i - x_j) \\ & + \sum_{i \in \pi_2, j \in \pi_1} \mathbb{1}_{\bar{\mathcal{C}}_j} \frac{1}{2} U_{1,2}(x_i - x_j) + \sum_{i,j \in \pi_2} \mathbb{1}_{\bar{\mathcal{C}}_j} \frac{1}{2} U_{2,2}(x_i - x_j). \end{aligned}$$

4. Derivation of the Gross-Pitaevskii Equation for a Class of Non Purely Positive Potentials

Consequently, $U_{\alpha,\beta}$ denotes the interaction potential between particles in π_α and π_β . Note that

$$\begin{aligned}
-\sum_P \sum_{j \in \pi_1} \Delta_j \mathbb{1}_{\bar{\mathcal{C}}_j} &= -\sum_{j=1}^N \Delta_j \mathbb{1}_{\bar{\mathcal{C}}_j} \frac{1}{2} \sum_P, \\
\sum_P \sum_{i,j \in \pi_1} \mathbb{1}_{\bar{\mathcal{C}}_j} U_{1,1}(x_i - x_j) &= \sum_P \sum_{i,j \in \pi_2} \mathbb{1}_{\bar{\mathcal{C}}_j} U_{2,2}(x_i - x_j) \\
&= \sum_{i \neq j=1}^N \mathbb{1}_{\bar{\mathcal{C}}_j} U^+(x_i - x_j) \frac{1}{4} \sum_P, \\
\sum_P \sum_{i \in \pi_1, j \in \pi_2} \mathbb{1}_{\bar{\mathcal{C}}_j} U_{1,2}(x_i - x_j) &= \\
&= \sum_{i \neq j=1}^N \mathbb{1}_{\bar{\mathcal{C}}_j} (2U^+(x_i - x_j) - 4U^-(x_i - x_j)) \frac{1}{4} \sum_P.
\end{aligned}$$

Therefore,

$$H_{\bar{\mathcal{C}}} = \sum_P H_P / \sum_P 1. \quad (4.47)$$

Hence, for N even, to obtain $H_{\bar{\mathcal{C}}} \geq 0$, it is sufficient to prove that for $\forall P$, $H_P \geq 0$.

If N is odd, we divide $P = (\pi_2, \pi_2)$, with $N_1 = (N-1)/2$ integers in π_1 and $(N+1)/2$ integers in π_2 .

Let A_j be a one-particle operator and define, for any partition $P = (\pi_1, \pi_2)$, $\delta_{j \in \pi_1}$ such that $\delta_{j \in \pi_1} = 1$ if $j \in \pi_1$, otherwise 0. Then $\sum_P \sum_{j \in \pi_1} A_j = \sum_{j=1}^N A_j \sum_P \delta_{j \in \pi_1}$. Note that

$$\sum_P \delta_{j \in \pi_1} = \frac{\sum_P \delta_{j \in \pi_1}}{\sum_P} \sum_P = \frac{\binom{N-1}{\frac{N-3}{2}}}{\binom{N}{\frac{N-1}{2}}} \sum_P = \frac{1 - \frac{1}{N}}{2} \sum_P.$$

Furthermore, for any two-particle operator $A_{i,j}$, we obtain, for $a, b \in \{1, 2\}$,

$$\sum_P \sum_{i \in \pi_a, j \in \pi_b, i \neq j} A_{i,j} = \sum_{i \neq j=1}^N A_{i,j} \sum_P \delta_{i \in \pi_a} \delta_{j \in \pi_b}.$$

Let $i \neq j$. With

$$\begin{aligned}
\frac{1}{\sum_P} \sum_P \delta_{i \in \pi_1} \delta_{j \in \pi_1} &= \frac{\binom{N-2}{\frac{N-5}{2}}}{\binom{N}{\frac{N-1}{2}}} = \frac{1}{4} \left(1 - \frac{3}{N} \right), & \frac{1}{\sum_P} \sum_P \delta_{i \in \pi_1} \delta_{j \in \pi_2} &= \frac{\binom{N-2}{\frac{N-3}{2}}}{\binom{N}{\frac{N-1}{2}}} = \frac{1}{4} \left(1 + \frac{1}{N} \right), \\
\frac{1}{\sum_P} \sum_P \delta_{i \in \pi_2} \delta_{j \in \pi_1} &= \frac{\binom{N-2}{\frac{N-3}{2}}}{\binom{N}{\frac{N-1}{2}}} = \frac{1}{4} \left(1 + \frac{1}{N} \right), & \frac{1}{\sum_P} \sum_P \delta_{i \in \pi_2} \delta_{j \in \pi_2} &= \frac{\binom{N-2}{\frac{N-1}{2}}}{\binom{N}{\frac{N-1}{2}}} = \frac{1}{4} \left(1 + \frac{1}{N} \right),
\end{aligned}$$

it follows that

$$\begin{aligned}
-\sum_P \sum_{j \in \pi_1} \Delta_j \mathbb{1}_{\bar{C}_j} &= -\frac{1 - \frac{1}{N}}{2} \sum_{j=1}^N \Delta_j \mathbb{1}_{\bar{C}_j} \sum_P, \\
\sum_P \sum_{i,j \in \pi_1} \mathbb{1}_{\bar{C}_j} U_{1,1}(x_i - x_j) &= \frac{1}{4} \left(1 - \frac{3}{N}\right) \sum_{i \neq j=1}^N \mathbb{1}_{\bar{C}_j} U^+(x_i - x_j) \sum_P, \\
\sum_P \sum_{i,j \in \pi_2} \mathbb{1}_{\bar{C}_j} U_{2,2}(x_i - x_j) &= \frac{1}{4} \left(1 + \frac{1}{N}\right) \sum_{i \neq j=1}^N \mathbb{1}_{\bar{C}_j} U^+(x_i - x_j) \sum_P, \\
\sum_P \sum_{i \in \pi_1, j \in \pi_2} \mathbb{1}_{\bar{C}_j} U_{1,2}(x_i - x_j) &= \frac{1}{4} \left(1 + \frac{1}{N}\right) \sum_{i \neq j=1}^N \mathbb{1}_{\bar{C}_j} U_{1,2}(x_i - x_j) \sum_P.
\end{aligned}$$

For N odd and N large enough, the bound of $H_P \geq 0$, $\forall P$ then implies, together with the Assumption 4.2.3 on U , that $H_{\bar{C}} \geq 0$.

We will now prove $H_P \geq 0$, $\forall P$. The advantage to consider H_P instead of $H_{\bar{C}}$ is that we can analyze $H_P \geq 0$ for fixed configurations of x_i 's with $i \in \pi_2$. This pointwise estimate is sufficient, since there is no kinetic energy of the π_2 -particles. Since permutation of the labels in π_1 and π_2 is irrelevant, we can further assume that $\pi_1 = \{1, \dots, N_1\}$, $\pi_2 = \{N_1 + 1, \dots, N\}$.

Following the idea of [72], for any fixed configuration (x_{N_1+1}, \dots, x_N) , we consider two cases:

- If there are more than m_1 π_2 -particles in a sphere of radius R with $m_1 \geq 2n_1$, the positive interaction $U_{2,2}$, together with $U_{1,1}$ cancels the negative part of $U_{1,2}$. Recall that n_1 is the number of cubes (or rectangles, respectively) of side length r_1/\sqrt{d} which are needed to cover a sphere of radius R . Therefore, if m_2 π_2 -particles are located in such a sphere, it is possible to derive that at least $\mathcal{O}(m_2^2/n_1)$ π_2 -particles are closer than r_1 to each other. Therefore, if m_1 π_1 -particles and m_2 π_2 -particles are close to each other, the potential energy is of order $\mathcal{O}(m_1^2) + \mathcal{O}(m_2^2) - \mathcal{O}(m_1 m_2)$. This energy is positive, if the negative part of U is small enough.
- If there are less than $2n_1$ π_2 -particles in a sphere of radius R , it is possible to use Assumption 4.2.3, (4.9), that is

$$-\mathbb{1}_{|x| \leq R} \Delta_x + n_1 (2U^+(x) - 4U^-(x)) \geq 0.$$

As in Definition 4.2.2, we divide \mathbb{R}^d into cubes C_n ($n \in \mathbb{N}$) of side length $\frac{1}{\sqrt{d}}r_1$, such that the distance between points $x_i, x_j \in C_n$ is not greater than r_1 . Therefore, for $x_i, x_j \in C_n$ we have by assumption $U(x_i - x_j) \geq \lambda^+$. Next, for fixed x_i , $i \in \pi_2$, for

any $x \in \mathbb{R}^d$, we define $G(x)$ as the set of i 's which satisfy $i \in \pi_2$ and $|x_i - x| \leq R$, i.e.,

$$G(x) \equiv \{i \in \pi_2 : |x_i - x| \leq R\}. \quad (4.48)$$

We denote $|G(x)|$ as the number of the elements of $G(x)$. Note that for $i, j \in G(x)$, it follows that $|x_i - x_j| \leq 2R$.

We denote $d(x, C_n)$ as the distance between the cube $C_n \subset \mathbb{R}^d$ and $x \in \mathbb{R}^d$. Since $|G(y)|$ is uniformly bounded ($|G(y)| \leq N_1$), there must exist a point $X(C_n) \in \mathbb{R}^d$ satisfying $d(X(C_n), C_n) \leq 2R$ and

$$|G(X(C_n))| = \max\{|G(y)| : d(y, C_n) \leq 2R\}. \quad (4.49)$$

We define $G(C_n) \equiv G(X(C_n))$. Let $\mathbb{1}_{C_n}(x_j)$ denote the projection onto C_n in the coordinate x_j . Furthermore, let Θ denote the usual Heaviside step function. We prove

$$\begin{aligned} \mathcal{H}_1 &= \sum_{i,j \in \pi_2} \mathbb{1}_{\bar{C}_j} U_{2,2}(x_i - x_j) + \sum_{i,j \in \pi_1} \mathbb{1}_{\bar{C}_j} U_{1,1}(x_i - x_j) \\ &\quad - \sum_{n \in \mathbb{N}} \Theta(|G(C_n)| - 2n_1) \sum_{j \in \pi_1, i \in \pi_2} \mathbb{1}_{C_n}(x_j) \mathbb{1}_{\bar{C}_j} U_{1,2}^-(x_i - x_j) \geq 0 \\ \mathcal{H}_{2,j} &= -2\Delta_j \mathbb{1}_{\bar{C}_j} + \sum_{i \in \pi_2} \mathbb{1}_{\bar{C}_j} \frac{1}{2} U_{1,2}^+(x_i - x_j) \\ &\quad - \sum_{n \in \mathbb{N}} \Theta(2n_1 - |G(C_n)|) \sum_{i \in \pi_2} \mathbb{1}_{C_n}(x_j) \mathbb{1}_{\bar{C}_j} \frac{1}{2} U_{1,2}^-(x_i - x_j) \geq 0. \end{aligned}$$

Note that this implies $H_p \geq 0$, since $H_p = \frac{1}{2}\mathcal{H}_1 + \sum_{j \in \pi_1} \mathcal{H}_{2,j}$.

Proof of $\mathcal{H}_1 \geq 0$:

First, we derive the lower bound on the total energy of $U_{2,2}$. With the definition of $G(C_n) = G(X(C_n))$, we know that the set $\{x_k : k \in G(C_n)\}$ can be covered by a sphere of radius R . So the number of the cubes which one need to cover this set is less than n_1 . We denote these cubes as $C_{n_1} \cdots C_{n_m}$ ($m \leq n_1$) and assume the number of i 's satisfying $i \in G(C_n)$ and $x_i \in C_{n_k}$ is a_{n_k} . Because the side length of C_{n_k} is equal to r_1/\sqrt{d} , the distance between the two particles in the same cube is no more than r_1 . Hence, we obtain, for $i \neq j$,

$$\sum_{i,j \in G(C_n)} \theta_{r_1}(x_i - x_j) \geq \sum_{k=1}^m \sum_{i,j \in C_{n_k}} = \sum_{k=1}^m [(a_{n_k})^2 - (a_{n_k})] \quad \text{and} \quad \sum_{k=1}^m a_{n_k} = |G(C_n)|.$$

Using Jensen's inequality, together with $m \leq n_1$,

$$\sum_{i,j \in G(C_n)} \theta_{r_1}(x_i - x_j) \geq \frac{1}{2n_1} |G(C_n)|^2.$$

Note that for fixed $i \in \pi_2$, the number of cubes C_n , which satisfy $i \in G(C_n)$ is less than n_2 . Since $U_{2,2}$ is nonnegative, we then obtain

$$\begin{aligned} \sum_{i,j \in \pi_2} \mathbb{1}_{\bar{C}_j} U_{2,2}(x_i - x_j) &= \sum_{n \in \mathbb{N}} \sum_{i,j \in \pi_2} \mathbb{1}_{C_n}(x_i) \mathbb{1}_{\bar{C}_j} U_{2,2}(x_i - x_j) \\ &\geq \frac{1}{n_2} \sum_{n \in \mathbb{N}} \sum_{i,j \in \pi_2, i \in G(C_n)} \mathbb{1}_{\bar{C}_j} U_{2,2}(x_i - x_j) \\ &\geq \frac{1}{n_2} \sum_{n \in \mathbb{N}} \Theta(|G(C_n)| - 2n_1) \sum_{i,j \in G(C_n)} \mathbb{1}_{\bar{C}_j} U_{2,2}(x_i - x_j). \end{aligned}$$

Since $r_1 < R$, it also follows that $n_1 \geq 2$. We then obtain $\mathbb{1}_{\bar{C}_j} U_{2,2}(x_i - x_j) = U_{2,2}(x_i - x_j)$, whenever $i, j \in G(C_n)$ with $|G(C_n)| \geq 2n_1$. Using $U_{2,2}(x) \geq \lambda^+ \Theta_{r_1}(x_i - x_j)$, we have with the estimates above

$$\sum_{i,j \in \pi_2} \mathbb{1}_{\bar{C}_j} U_{2,2}(x_i - x_j) \geq \sum_{n \in \mathbb{N}} \Theta(|G(C_n)| - 2n_1) \frac{\lambda^+}{2n_1 n_2} |G(C_n)|^2.$$

Next, we derive the lower bound on the interaction potential between particles in π_1 . Let $\Pi_1(C_n)$ be defined as the set of i 's such that $i \in \pi_1$ and $x_i \in C_n$. Let $|\Pi_1(C_n)|$ denote the number of the elements of $\Pi_1(C_n)$. If $x_i \in C_n$ and $|G(C_n)| \geq 1$, there must be a $k \in \pi_2$ satisfying $|x_i - x_k| \leq 2R$. Thus, for any C_n we have that

$$\begin{aligned} \sum_{i,j \in \pi_1} \mathbb{1}_{\bar{C}_j} U_{1,1}(x_i - x_j) &= \sum_{n \in \mathbb{N}} \sum_{i,j \in \pi_1} \mathbb{1}_{C_n}(x_i) \mathbb{1}_{\bar{C}_j} U_{1,1}(x_i - x_j) \\ &\geq \sum_{n \in \mathbb{N}} \Theta(|G(C_n)| - 2n_1) \sum_{i,j \in \Pi_1(C_n)} U_{1,1}(x_i - x_j). \end{aligned}$$

For $i, j \in \Pi_1(C_n)$, $i \neq j$, the distance between x_i and x_j is not more than r_1 . Hence,

$$\sum_{i,j \in \Pi_1(C_n)} U_{1,1}(x_i - x_j) \geq \lambda^+ \left(|\Pi_1(C_n)|^2 - |\Pi_1(C_n)| \right). \quad (4.50)$$

At last, we derive the lower bound on $U_{1,2}^-$.

By the definitions of $|G(C_n)|$ and $U_{1,2}$, we have that $\forall x \in C_n$,

$$-\sum_{i \in \pi_2} U_{1,2}^-(x - x_i) \geq -4\lambda^- |G(C_n)|.$$

This yields to

$$-\sum_{j \in \Pi_1(C_n), i \in \pi_2} \mathbb{1}_{\bar{C}_j} U_{2,1}^-(x_i - x_j) \geq -4\lambda^- |\Pi_1(C_n)| |G(C_n)|. \quad (4.51)$$

We now consider

$$\begin{aligned} & \sum_{i,j \in \Pi_1(C_n)} U_{1,1}(x_i - x_j) - \sum_{j \in \Pi_1(C_n), i \in \pi_2} \mathbb{1}_{\bar{C}_j} U_{1,2}^-(x_i - x_j) \\ & \geq \lambda^+ \left(|\Pi_1(C_n)|^2 - |\Pi_1(C_n)| \right) - 4\lambda^- |\Pi_1(C_n)| |G(C_n)|. \end{aligned} \quad (4.52)$$

Using $\lambda^- \leq \frac{1}{8n_2} \lambda^+$, we then obtain for $|G(C_n)| \geq n_1$

$$(4.52) \geq \lambda^+ \left(|\Pi_1(C_n)|^2 - |\Pi_1(C_n)| - \frac{1}{2n_2} |\Pi_1(C_n)| |G(C_n)| \right).$$

If $|\Pi_1(C_n)| = 1$, we obtain for $|G(C_n)| \geq 2n_1$

$$(4.52) \geq -\lambda^+ \frac{|G(C_n)|^2}{4n_1 n_2}.$$

For $|\Pi_1(C_n)| \geq 2$, we have $|\Pi_1(C_n)|^2 - |\Pi_1(C_n)| \geq \frac{1}{2} |\Pi_1(C_n)|^2$ and therefore, for $|G(C_n)| \geq 2n_1$

$$(4.52) \geq \frac{\lambda^+}{2} \left(|\Pi_1(C_n)|^2 - 2|\Pi_1(C_n)| \frac{1}{2n_2} |G(C_n)| \right) \geq -\frac{\lambda^+}{2} \frac{1}{4(n_2)^2} |G(C_n)|^2.$$

Since $n_2 \geq n_1$ holds, we then obtain for $|G(C_n)| \geq 2n_1$ and for all $|\Pi_1(C_n)| \in \mathbb{N}$

$$(4.52) \geq -\lambda^+ \frac{|G(C_n)|^2}{4n_1 n_2}.$$

Therefore, we obtain

$$\mathcal{H}_1 \geq \sum_{n \in \mathbb{N}} \Theta(|G(C_n)| - 2n_1) \left(\frac{\lambda^+}{2n_1 n_2} |G(C_n)|^2 - \frac{\lambda^+}{4n_1 n_2} |G(C_n)|^2 \right) \geq 0.$$

Proof of $\mathcal{H}_{2,j} \geq 0$:

Since there is no kinetic energy for the π_2 particles, we prove $\mathcal{H}_{2,j} \geq 0$ for fixed $x_i, i \in \pi_2$. Define

$$\tilde{\mathcal{H}}_{2,j} = -2\Delta_j + \sum_{i \in \pi_2} \frac{1}{2} U_{1,2}^+(x_i - x_j) - \sum_{n \in \mathbb{N}} \Theta(2n_1 - |G(C_n)|) \sum_{i \in \pi_2} \mathbb{1}_{C_n}(x_j) \frac{1}{2} U_{1,2}^-(x_i - x_j) \quad (4.53)$$

Note that

$$\mathcal{H}_{2,j} = \mathbb{1}_{\bar{C}_j} \tilde{\mathcal{H}}_{2,j}$$

and $\mathbb{1}_{\bar{C}_j}$ commutes with $-\Delta_j$. Hence, it suffices to prove $\tilde{\mathcal{H}}_{2,j} \geq 0$. Let

$$\pi'_2 = \{i \in \pi_2 : \exists C_n, D(x_i, C_n) \leq R, |G(C_n)| \leq 2n_1\}.$$

For fixed x_i and x_j , if

$$\Theta(2n_1 - |G(C_n)|) \mathbb{1}_{C_n}(x_j) \frac{1}{2} U_{1,2}^-(x_i - x_j) \neq 0,$$

it then follows $i \in \pi'_2$. Therefore,

$$\sum_{n \in \mathbb{N}} \Theta(2n_1 - |G(C_n)|) \sum_{i \in \pi_2} \frac{1}{2} \mathbb{1}_{C_n}(x_j) U_{1,2}^-(x_i - x_j) \leq \sum_{i \in \pi'_2} \frac{1}{2} U_{1,2}^-(x_i - x_j).$$

Since $\pi'_2 \subset \pi_2$, it follows that

$$(4.53) \geq -2\Delta_j + \sum_{i \in \pi'_2} \frac{1}{2} (U_{1,2}^+(x_i - x_j) - U_{1,2}^-(x_i - x_j)).$$

By the definition of π'_2 , it follows that for any $x \in \mathbb{R}^d$

$$\sum_{i \in \pi'_2} \mathbb{1}_{|x_i - x| \leq R} \leq 2n_1.$$

Under the assumptions on U , we obtain

$$(4.53) \geq \frac{1}{n_1} \sum_{i \in \pi'_2} \left(-\mathbb{1}_{|x_i - x_j| \leq R} \Delta_j + \frac{n_1}{2} U_{1,2}(x_i - x_j) \right) \geq 0.$$

□

Corollary 4.3.15 *Let V fulfill Assumption 4.2.3. Then, there exists a constant $0 < \epsilon < 1$ such that*

(a) *For $d = 3$,*

$$-\sum_{k=1}^N \Delta_k + \sum_{i < j=1}^N (V_1^+(x_i - x_j) - (1 + \epsilon) V_1^-(x_i - x_j)) \geq 0, \quad (4.54)$$

$$(1 - \epsilon) \sum_{k=1}^N -\Delta_k \mathbb{1}_{\bar{B}_k} + \sum_{i \neq j} \mathbb{1}_{\bar{B}_j} \frac{1}{2} V_1(x_i - x_j) \geq 0. \quad (4.55)$$

(b) *For $d = 2$, with $V_N(x) = e^{2N} V(e^N x)$ and $\bar{B}_j^{(d)}$ defined as in Definition 3.5.4,*

$$-\sum_{k=1}^N \Delta_k + \sum_{i < j=1}^N (V_N^+(x_i - x_j) - (1 + \epsilon) V_N^-(x_i - x_j)) \geq 0, \quad (4.56)$$

$$(1 - \epsilon) \sum_{k=1}^N -\Delta_k \mathbb{1}_{\bar{B}_k^{(d)}} + \sum_{i \neq j} \mathbb{1}_{\bar{B}_j^{(d)}} \frac{1}{2} V_N(x_i - x_j) \geq 0. \quad (4.57)$$

Remark 4.3.16 *These operator inequalities are crucial in order to prove Conditions (4.19), (4.20) and (4.21), see below. We do not except the persistence of condensation if (4.54) and (4.55) were not true. In that case, one would rather expect the condensate to collapse in the limit $N \rightarrow \infty$ in finite time.*

Proof: By rescaling $Nx \rightarrow x$, the first inequality (4.54) is equivalent to $-\sum_{k=1}^N \Delta_k + \sum_{i < j=1}^N (V^+(x_i - x_j) - (1 + \epsilon)V^-(x_i - x_j)) \geq 0$. Setting $U(x) = V^+(x) - (1 + \epsilon)V^-(x)$, U then fulfills the conditions of Lemma 4.3.10 which implies the inequality above.

Setting $\bar{\mathcal{D}}_j := \bigcup_{k,l \neq j} \{(x_1, x_2, \dots, x_N) \in \mathbb{R}^{3N} : |x_l - x_k| < NN^{-26/27}\}$, the second inequality is equivalent to

$$(1 - \epsilon) \sum_{k=1}^N -\Delta_k \mathbb{1}_{\bar{\mathcal{D}}_k} + \sum_{i \neq j} \mathbb{1}_{\bar{\mathcal{D}}_j} \frac{1}{2} V(x_i - x_j) \geq 0.$$

Note that the set $\bar{\mathcal{D}}_j$ defined above fulfills $\tilde{R} = N^{1/27} > 2R$. Hence, Lemma 4.3.13, part (b) implies the second inequality (4.55), setting $U = \frac{1}{1-\epsilon}V$. In the same manner, we obtain part (b) of the Lemma, rescaling $e^N x \rightarrow x$. For this, note that the rescaled set

$$e^N \bar{\mathcal{B}}_j^{(d)} = \bigcup_{k \neq l \neq j} a_{k,l}^{(d)} = \bigcup_{k,l \neq j} \{(x_1, x_2, \dots, x_N) \in \mathbb{R}^{2N} : |x_k - x_l| < e^N N^{-d}\} \quad (4.58)$$

is such that $e^N N^{-d} > 2R$ for all $d \in \mathbb{N}$ for N large enough. Hence, Lemma 4.3.13, part (b) can be applied.

□

4.3.3 Proof of Conditions (4.19) and (4.20)

Lemma 4.3.17 *Let $d = 3$, let V fulfill Assumption 4.2.3 and let $A_t \in L^\infty(\mathbb{R}^3, \mathbb{R})$. Then, for all $\Psi \in L_s^2(\mathbb{R}^{3N}, \mathbb{C}) \cap H^2(\mathbb{R}^{3N}, \mathbb{C})$*

(a)

$$\|V_1(x_1 - x_2)\Psi\|^2 \leq C \langle\langle \Psi, H\Psi \rangle\rangle + CN. \quad (4.59)$$

(b)

$$\|\nabla_1 \Psi\|^2 \leq \frac{C}{N} (\langle\langle \Psi, H\Psi \rangle\rangle + 1). \quad (4.60)$$

Proof:

(a) Let, for $0 < \epsilon < 1$,

$$H^{(\epsilon)} = -\sum_{k=1}^N \Delta_k + \sum_{i < j} (V_1^+(x_i - x_j) - (1 + \epsilon)V_1^-(x_i - x_j)) + \sum_{k=1}^N A.(x_k).$$

Since V fulfills Assumption 4.2.3, Corollary 4.3.15 implies together with $A. \in L^\infty(\mathbb{R}^3, \mathbb{R})$, $H^{(\epsilon)} \geq -CN$. We then obtain

$$\epsilon \sum_{i < j=1}^N V_1^-(x_i - x_j) \leq H + CN.$$

Furthermore

$$\sum_{i < j=1}^N V_1^+(x_i - x_j) \leq H + \sum_{i < j=1}^N V_1^-(x_i - x_j) + N\|A.\|_\infty \leq \left(1 + \frac{1}{\epsilon}\right) H + CN.$$

Thus,

$$\begin{aligned} \|V_1(x_1 - x_2)\Psi\|^2 &\leq \|V_1\|_\infty (\langle\langle \Psi, V_1^+(x_1 - x_2)\Psi \rangle\rangle + \langle\langle \Psi, V_1^-(x_1 - x_2)\Psi \rangle\rangle) \\ &\leq C \left(\langle\langle \Psi, \sum_{i < j=1}^N V_1^+(x_i - x_j)\Psi \rangle\rangle + \langle\langle \Psi, \sum_{i < j=1}^N V_1^-(x_i - x_j)\Psi \rangle\rangle \right) \\ &\leq C\langle\langle \Psi, H\Psi \rangle\rangle + CN. \end{aligned}$$

(b) We use

$$-CN \leq H^{(\epsilon)} \leq (1 + \epsilon) \left(\frac{-1}{1 + \epsilon} \sum_{k=1}^N \Delta_k + \sum_{i < j} V_1(x_i - x_j) + \sum_{k=1}^N \frac{1}{1 + \epsilon} A_t(x_k) \right).$$

Let $\mu = 1 - \frac{1}{1 + \epsilon} > 0$. Using $A. \in L^\infty(\mathbb{R}^d, \mathbb{R})$, we then obtain

$$-\mu \sum_{k=1}^N \Delta_k \leq H + CN.$$

□

Remark 4.3.18 Lemma 4.3.17, part (a) can also be derived from part (b), using Sobolev's inequality

$$\begin{aligned} &|\langle\langle \Psi, V_1^2(x_1 - x_2)\Psi \rangle\rangle| \\ &\leq \|V_1\|_\infty^2 \|\mathbb{1}_{B_{N^{-1}}(0)}\|_{\frac{3}{2}}^{\frac{3}{2}} \int dx_2 \cdots \int dx_N \left(\int dx_1 |\Psi(x_1, \dots, x_N)|^6 \right)^{1/3} \\ &\leq CN^4 N^{-2} \|\nabla_1 \Psi\|^2 \leq C(\langle\langle \Psi_t, H\Psi_t \rangle\rangle + N). \end{aligned}$$

Using Lemma 4.3.17 together with $\frac{\langle\langle \Psi_t, H\Psi_t \rangle\rangle}{N} \leq C$, we then prove Conditions (4.19) and (4.20).

Corollary 4.3.19 *Let $d = 2$ and let V fulfill Assumption 4.2.3. Let $V_N(x) = e^{2N}V(e^N x)$ and let H_{V_N} be defined as in (3.2) with $A_t \in L^\infty(\mathbb{R}^2, \mathbb{R})$. Then, for all $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap H^2(\mathbb{R}^{2N}, \mathbb{C})$*

$$\|\nabla_1 \Psi\|^2 \leq \frac{C}{N} (\langle\langle \Psi, H_{V_N} \Psi \rangle\rangle + 1). \quad (4.61)$$

Proof: The proof of Lemma 4.3.17, part (b) can be straightforwardly be applied in the two dimensional case. □

4.3.4 Proof of Condition (4.21)

We will first restate a Lemma which we will need in the following.

Proposition 4.3.20 *Let $\Omega \in H^1(\mathbb{R}^{3N}, \mathbb{C})$. Then, for all $j \neq k$*

$$\|\mathbb{1}_{\bar{B}_j} \Omega\| \leq C N^{-7/54} \|\nabla_j \Omega\|.$$

Proof: The proof of this Lemma, which is a direct consequence of Sobolev's inequality, can be found in [60], Proposition A.1. □

Lemma 4.3.21 *Assume V fulfills Assumption 4.2.3. Then, for any $\Psi \in L_s^2(\mathbb{R}^{3N}, \mathbb{C}) \cap H^2(\mathbb{R}^{3N}, \mathbb{C})$ and any $\varphi \in H^2(\mathbb{R}^3, \mathbb{C})$ there exists a $\eta > 0$ such that*

(a)

$$\|\mathbb{1}_{\mathcal{A}_1} \nabla_1 q_1 \Psi\|^2 \leq C (\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + N^{-\eta}) + |\mathcal{E}(\Psi) - \mathcal{E}^{GP}(\varphi)|.$$

(b)

$$\|\mathbb{1}_{\bar{B}_1} \nabla_1 \Psi\|^2 \leq C (\langle\langle \Psi, \widehat{n} \Psi \rangle\rangle + N^{-\eta}) + |\mathcal{E}(\Psi) - \mathcal{E}^{GP}(\varphi)|.$$

Remark 4.3.22 *For nonnegative potentials, the proof of Lemma 4.3.21 was given in Lemma 5.2. in [60]. For potentials which fulfill Assumption 4.2.3 we use Corollary 4.3.15 in order to obtain the same bound.*

Proof: Let us first split up the energy difference. Since $\Psi \in L_s^2(\mathbb{R}^{3N}, \mathbb{C})$ is symmetric,

$$\begin{aligned} \mathcal{E}(\Psi) - \mathcal{E}^{GP}(\varphi) &= \|\nabla_1 \Psi\|^2 + (N-1) \langle\langle \Psi, V_1(x_1 - x_2) \Psi \rangle\rangle \\ &\quad - \|\nabla \varphi\|^2 - 2a \|\varphi^2\|^2 + \langle\langle \Psi, A \cdot \Psi \rangle\rangle - \langle \varphi, A \cdot \varphi \rangle\rangle. \end{aligned}$$

Let W_{β_1} be defined as in Lemma 4.3.7 for some β_1 . Then,

$$\begin{aligned}\mathcal{E}(\Psi) - \mathcal{E}^{GP}(\varphi) &= \|\mathbf{1}_{\mathcal{A}_1} \nabla_1 \Psi\|^2 + \|\mathbf{1}_{\bar{\mathcal{B}}_1} \mathbf{1}_{\bar{\mathcal{A}}_1} \nabla_1 \Psi\|^2 + \|\mathbf{1}_{\mathcal{B}_1} \mathbf{1}_{\bar{\mathcal{A}}_1} \nabla_1 \Psi\|^2 \\ &\quad + (N-1) \langle \langle \Psi, \mathbf{1}_{\bar{\mathcal{B}}_1} V_1 (x_1 - x_2) \Psi \rangle \rangle \\ &\quad + \langle \langle \Psi, \sum_{j \neq 1} \mathbf{1}_{\mathcal{B}_1} (V_1 - W_{\beta_1}) (x_1 - x_j) \Psi \rangle \rangle \\ &\quad + \langle \langle \Psi, \sum_{j \neq 1} \mathbf{1}_{\mathcal{B}_1} W_{\beta_1} (x_1 - x_j) \Psi \rangle \rangle - \|\nabla \varphi\|^2 - 2a \|\varphi^2\|^2 \\ &\quad + \langle \langle \Psi A \cdot \Psi \rangle \rangle - \langle \varphi A \cdot \varphi \rangle.\end{aligned}$$

Using that $q_1 = 1 - p_1$, we obtain for $0 < \epsilon < 1$,

$$\mathcal{E}(\Psi) - \mathcal{E}^{GP}(\varphi) = \epsilon \left(\|\mathbf{1}_{\mathcal{A}_1} \nabla_1 q_1 \Psi\|^2 + \|\mathbf{1}_{\bar{\mathcal{B}}_1} \mathbf{1}_{\bar{\mathcal{A}}_1} \nabla_1 \Psi\|^2 \right) \quad (4.62)$$

$$+ 2\Re(\langle \nabla_1 q_1 \Psi, \mathbf{1}_{\mathcal{A}_1} \nabla_1 p_1 \Psi \rangle) \quad (4.63)$$

$$+ \|\mathbf{1}_{\mathcal{B}_1} \mathbf{1}_{\bar{\mathcal{A}}_1} \nabla_1 \Psi\|^2 + \frac{1}{2} \langle \langle \Psi, \sum_{j=2}^N \mathbf{1}_{\mathcal{B}_1} (V_1 - W_{\beta_1}) (x_1 - x_j) \Psi \rangle \rangle \quad (4.64)$$

$$+ \frac{N-1}{2} \langle \langle \Psi, \mathbf{1}_{\mathcal{B}_1} p_1 p_2 W_{\beta_1} (x_1 - x_2) p_1 p_2 \mathbf{1}_{\mathcal{B}_1} \Psi \rangle \rangle - \frac{a}{2} \|\varphi^2\|^2 \quad (4.65)$$

$$+ (N-1) \Re(\langle \Psi, \mathbf{1}_{\mathcal{B}_1} (1 - p_1 p_2) W_{\beta_1} (x_1 - x_2) p_1 p_2 \mathbf{1}_{\mathcal{B}_1} \Psi \rangle) \quad (4.66)$$

$$+ \frac{N-1}{2} \langle \langle \Psi, \mathbf{1}_{\mathcal{B}_1} (1 - p_1 p_2) W_{\beta_1} (x_1 - x_2) (1 - p_1 p_2) \mathbf{1}_{\mathcal{B}_1} \Psi \rangle \rangle \quad (4.67)$$

$$+ \|\mathbf{1}_{\mathcal{A}_1} \nabla_1 p_1 \Psi\|^2 - \|\nabla \varphi\|^2 \quad (4.68)$$

$$+ \langle \langle \Psi, A \cdot (x_1) \Psi \rangle \rangle - \langle \varphi, A \cdot \varphi \rangle \quad (4.69)$$

$$+ (1 - \epsilon) \left(\|\mathbf{1}_{\mathcal{A}_1} \nabla_1 q_1 \Psi\|^2 + \|\mathbf{1}_{\bar{\mathcal{B}}_1} \mathbf{1}_{\bar{\mathcal{A}}_1} \nabla_1 \Psi\|^2 \right) \quad (4.70)$$

$$+ \frac{N-1}{2} \langle \langle \Psi, \mathbf{1}_{\bar{\mathcal{B}}_1} V_1 (x_1 - x_2) \Psi \rangle \rangle. \quad (4.71)$$

It has been shown in [60] that for some suitable chosen $0 < \beta_1 < 1$ there exists an $\eta > 0$ such that

$$|(4.62)| + |(4.63)| + |(4.65)| + |(4.68)| + |(4.69)| \leq C \left(\langle \Psi, \widehat{n} \Psi \rangle + N^{-\eta} \right) + |\mathcal{E}(\Psi) - \mathcal{E}^{GP}(\varphi)|.$$

Since $(4.64) \geq 0$, $(4.66) \geq 0$, we are left to control (4.70) and (4.71) in order to show

$$\epsilon \left(\|\mathbf{1}_{\mathcal{A}_1} \nabla_1 q_1 \Psi\|^2 + \|\mathbf{1}_{\bar{\mathcal{B}}_1} \mathbf{1}_{\bar{\mathcal{A}}_1} \nabla_1 \Psi\|^2 \right) \leq C \left(\langle \Psi, \widehat{n} \Psi \rangle + N^{-\eta} \right) + |\mathcal{E}(\Psi) - \mathcal{E}^{GP}(\varphi)|.$$

For nonnegative potentials, the trivial bound $(4.70) + (4.71) \geq 0$ is sufficient in order to prove Lemma 4.3.21. For potentials fulfilling Assumption 4.2.3, we use

$$\begin{aligned}(4.70) + (4.71) &= (1 - \epsilon) \left(\|\mathbf{1}_{\mathcal{A}_1} \mathbf{1}_{\bar{\mathcal{B}}_1} \nabla_1 \Psi\|^2 + \|\mathbf{1}_{\bar{\mathcal{B}}_1} \mathbf{1}_{\bar{\mathcal{A}}_1} \nabla_1 \Psi\|^2 \right) + \frac{N-1}{2} \langle \langle \Psi, \mathbf{1}_{\bar{\mathcal{B}}_1} V_1 (x_1 - x_2) \Psi \rangle \rangle \\ &\quad - (1 - \epsilon) 2\Re(\langle \nabla_1 \Psi, \mathbf{1}_{\mathcal{A}_1} \mathbf{1}_{\bar{\mathcal{B}}_1} \nabla_1 p_1 \Psi \rangle) \\ &\quad + (1 - \epsilon) \left(\|\mathbf{1}_{\mathcal{A}_1} \mathbf{1}_{\mathcal{B}_1} \nabla_1 q_1 \Psi\|^2 + \|\mathbf{1}_{\mathcal{A}_1} \mathbf{1}_{\bar{\mathcal{B}}_1} \nabla_1 p_1 \Psi\|^2 \right).\end{aligned}$$

We will estimate each line separately. The third line is positive. Using Proposition 4.3.20, we obtain

$$\|\mathbb{1}_{\mathcal{A}_1} \mathbb{1}_{\bar{\mathcal{B}}_1} \nabla_1 p_1 \Psi\| \leq \|\mathbb{1}_{\bar{\mathcal{B}}_1} \nabla_1 p_1 \Psi\| \leq CN^{-7/54} \|\Delta_1 p_1 \Psi\|.$$

This implies for the second line

$$|2\Re(\langle \nabla_1 \Psi, \mathbb{1}_{\bar{\mathcal{B}}_1} \mathbb{1}_{\mathcal{A}_1} \nabla_1 p_1 \Psi \rangle)| \leq CN^{-7/54}.$$

Focusing on the first term, we obtain with Corollary 4.3.15

$$\begin{aligned} & (1-\epsilon) (\|\mathbb{1}_{\mathcal{A}_1} \mathbb{1}_{\bar{\mathcal{B}}_1} \nabla_1 \Psi\|^2 + \|\mathbb{1}_{\bar{\mathcal{B}}_1} \mathbb{1}_{\bar{\mathcal{A}}_1} \nabla_1 \Psi\|^2) + \frac{N-1}{2} \langle \Psi, \mathbb{1}_{\bar{\mathcal{B}}_1} V_1(x_1 - x_2) \Psi \rangle \\ &= \frac{1}{N} \langle \Psi, \left((1-\epsilon) \sum_{k=1}^N -\Delta_k \mathbb{1}_{\bar{\mathcal{B}}_k} + \sum_{i \neq j} \mathbb{1}_{\bar{\mathcal{B}}_j} \frac{1}{2} V_1(x_i - x_j) \Psi \right) \rangle \geq 0. \end{aligned}$$

We have therefore shown

$$\|\mathbb{1}_{\mathcal{A}_1} \nabla_1 q_1 \Psi\|^2 + \|\mathbb{1}_{\bar{\mathcal{B}}_1} \mathbb{1}_{\bar{\mathcal{A}}_1} \nabla_1 \Psi\|^2 \leq C (\langle \Psi, \hat{n} \Psi \rangle + N^{-\eta} + |\mathcal{E}(\Psi) - \mathcal{E}^{GP}(\varphi)|).$$

Note that

$$\begin{aligned} \|\mathbb{1}_{\bar{\mathcal{B}}_1} \nabla_1 q_1 \Psi\|^2 &= \|\mathbb{1}_{\bar{\mathcal{A}}_1} \mathbb{1}_{\bar{\mathcal{B}}_1} \nabla_1 q_1 \Psi\|^2 + \|\mathbb{1}_{\mathcal{A}_1} \mathbb{1}_{\bar{\mathcal{B}}_1} \nabla_1 q_1 \Psi\|^2 \\ &\leq \|\mathbb{1}_{\bar{\mathcal{A}}_1} \mathbb{1}_{\bar{\mathcal{B}}_1} \nabla_1 (1-p_1) \Psi\|^2 + \|\mathbb{1}_{\mathcal{A}_1} \nabla_1 q_1 \Psi\|^2 \\ &\leq 2 \|\mathbb{1}_{\bar{\mathcal{A}}_1} \mathbb{1}_{\bar{\mathcal{B}}_1} \nabla_1 \Psi\|^2 + 2 \|\mathbb{1}_{\bar{\mathcal{A}}_1} \mathbb{1}_{\bar{\mathcal{B}}_1} \nabla_1 p_1 \Psi\|^2 + \|\mathbb{1}_{\mathcal{A}_1} \nabla_1 q_1 \Psi\|^2. \end{aligned}$$

Using $\|\mathbb{1}_{\bar{\mathcal{B}}_1} \mathbb{1}_{\bar{\mathcal{A}}_1} \nabla_1 p_1 \Psi\| \leq \|\mathbb{1}_{\bar{\mathcal{B}}_1} \nabla_1 p_1 \Psi\| \leq CN^{-7/54} \|\Delta_1 p_1 \Psi\|$, we then obtain the Lemma. □

Chapter 5

Derivation of the Two Dimensional Focusing NLS Equation

Contributions of the author and Acknowledgments

This chapter presents joint work with Prof. Peter Pickl and has with minor modifications already been published as the preprint [26]. The preprint was written by me. My contribution to the conceptual ideas is 70 % and my share on their technical implementation is 80 %.

We are grateful to Dr. Nikolai Leopold for pointing out to us the idea to use the variance of the energy in our estimates and how to include time-dependent external potentials. We would like to thank Lea Boßmann for helpful discussions. We also would like to thank Dr. David Mitrouskas and an anonymous referee for various valuable comments on an earlier version of this result which led to improved estimates and an improved presentation. M.J. gratefully acknowledges financial support by the German National Academic Foundation.

5.1 Introduction

During the last decades, the experimental realization and the theoretical investigation of Bose-Einstein condensation (BEC) regained a considerable amount of attention. Mathematically, there is a steady effort to describe both the dynamical as well as the statical properties of such condensates. While the principal mechanism of BEC is similar for many different systems, the specific effective description of such a system depends strongly on the model one studies. In this chapter we will focus on a dilute, two dimensional system of bosons with attractive interaction.

Let us first define the N -body quantum problem we have in mind. The evolution of N interacting bosons is described by a time-dependent wave-function $\Psi_t \in L_s^2(\mathbb{R}^{2N}, \mathbb{C})$, $\|\Psi_t\| = 1$. Ψ_t solves the N -particle Schrödinger equation

$$i\partial_t \Psi_t = H_{W_\beta, t} \Psi_t, \quad (5.1)$$

where the time-dependent Hamiltonian $H_{W_\beta,t}$ is given by

$$H_{W_\beta,t} = - \sum_{j=1}^N \Delta_j + \sum_{1 \leq j < k \leq N} W_\beta(x_j - x_k) + \sum_{j=1}^N A_t(x_j). \quad (5.2)$$

The scaled potential $W_\beta(x) = N^{-1+2\beta} W(N^\beta x)$, $W \in L_c^\infty(\mathbb{R}^2, \mathbb{R})$ describes a strong, but short range potential acting on the length scale of order $N^{-\beta}$ (we assume W to be compactly supported). The external potential $A_t \in L^p(\mathbb{R}^2, \mathbb{R})$ for some $p > 1$ is used as an external trapping potential. Below, we will comment on different choices for A_t in more detail. In general, even for small particle numbers N , the evolution equation (5.1) cannot be solved directly nor numerically for Ψ_t . Nevertheless, for a certain class of initial conditions Ψ_0 and certain interactions W , which we will make precise in a moment, it is possible to derive an approximate solution of (5.1) in the trace class topology of reduced density matrices.

Recall the definition of the one particle reduced density matrix $\gamma_{\Psi_0}^{(1)}$ of Ψ_0 with integral kernel

$$\gamma_{\Psi_0}^{(1)}(x, x') = \int_{\mathbb{R}^{2N-2}} \Psi_0^*(x, x_2, \dots, x_N) \Psi_0(x', x_2, \dots, x_N) d^2 x_2 \dots d^2 x_N.$$

To account for the physical situation of a Bose-Einstein condensate, we assume complete condensation in the limit of large particle number N . This amounts to assume that, for $N \rightarrow \infty$, $\gamma_{\Psi_0}^{(1)} \rightarrow |\varphi_0\rangle\langle\varphi_0|$ in trace norm for some $\varphi_0 \in L^2(\mathbb{R}^2, \mathbb{C})$, $\|\varphi_0\| = 1$. Define $a = \int_{\mathbb{R}^2} d^2 x W(x)$ (throughout this chapter, a will always denote the integral over W). Let φ_t solve the nonlinear Schrödinger equation

$$i\partial_t \varphi_t = (-\Delta + A_t) \varphi_t + a|\varphi_t|^2 \varphi_t =: h_{a,t}^{\text{NLS}} \varphi_t \quad (5.3)$$

with initial datum φ_0 . Our main goal is to show the persistence of condensation over time. In particular, we prove that the time evolved reduced density matrix $\gamma_{\Psi_t}^{(1)}$ converges to $|\varphi_t\rangle\langle\varphi_t|$ in trace norm as $N \rightarrow \infty$ with convergence rate of order $N^{-\eta}$ for some explicitly computable $\eta > 0$, see Lemma 5.3.7. Assuming $W \in L_c^\infty(\mathbb{R}^2, \mathbb{R})$, such that W is spherically symmetric and $-(1-\epsilon)\Delta + \frac{1}{2}W \geq 0$ holds for some $\epsilon > 0$, the convergence $\gamma_{\Psi_t}^{(1)} \rightarrow |\varphi_t\rangle\langle\varphi_t|$ in trace norm for all $\beta > 0$ was shown in Chapter 3, see also [30] for a prior result. Recall that the operator inequality just stated implies $a > 0$, see e.g. [13]. The problem becomes more delicate for interactions which are more general, especially if (5.3) is focusing, which means $a < 0$. For strong, attractive potentials, it is known that the condensate collapses in the limit of large particle number. To prevent this behavior, our proof needs stability of second kind for the Hamiltonian $H_{W_\beta,t}$, that is, we assume $H_{W_\beta,t} \geq -CN$. If W_β is partly or purely nonpositive, this assumption gets highly nontrivial for higher β . For $\beta \leq 1/2$,

the inequality

$$\begin{aligned} & \inf_{\Psi \in L^2(\mathbb{R}^{2N}, \mathbb{C}), \|\Psi\|=1} \frac{\langle\langle \Psi, H_{W_\beta, t} \Psi \rangle\rangle}{N} \\ & \geq \inf_{\varphi \in L^2(\mathbb{R}^2, \mathbb{C}), \|\varphi\|=1} \left(\int_{\mathbb{R}^2} d^2x \left(|\nabla \varphi(x)|^2 + A_t(x)|\varphi(x)|^2 + \frac{1}{2} \int_{\mathbb{R}^2} d^2x |\varphi(x)|^2 (NW_\beta * |\varphi|^2)(x) \right) \right) \\ & \quad - o(1) - CN^{2\beta-1}, \end{aligned} \tag{5.4}$$

which was proven in [45], shows $H_{W_\beta, t} \geq -CN$, if (5.4), which is the ground state energy of the nonlinear Hartree functional, is bounded from below uniformly in N . Assuming $A_t \geq -C$, this is the case if

$$\inf_{\varphi \in H^1(\mathbb{R}^2, \mathbb{C})} \left(\frac{\int_{\mathbb{R}^2} d^2x |\varphi(x)|^2 (|\varphi|^2 * W)(x)}{\|\varphi\|^2 \|\nabla \varphi\|^2} \right) > -1 \tag{5.5}$$

holds [47]. Assuming Condition (5.5) together with $A_t \in L^1_{\text{loc}}(\mathbb{R}^2, \mathbb{R})$, $A_t(x) \geq C|x|^s$, $s > 0$, stability of second kind was subsequently proven for all $0 < \beta < \frac{s+1}{s+2}$ [47]. In particular, it was shown that the ground state energy per particle of $H_{W_\beta, t}$ is then given (in the limit $N \rightarrow \infty$) by the corresponding nonlinear Schrödinger functional; see also [46] for an earlier result which also treats the one- and three-dimensional cases.

Condition (5.5) thus restricts the set of interactions W . Indeed, stability of the second kind fails if

$$\inf_{\varphi \in H^1(\mathbb{R}^2, \mathbb{C})} \left(\frac{\int_{\mathbb{R}^2} d^2x |\varphi(x)|^2 (|\varphi|^2 * W)(x)}{\|\varphi\|^2 \|\nabla \varphi\|^2} \right) < -1, \tag{5.6}$$

see [46, 47] for a nice discussion. Let W^- denote the negative part of W and let $a^* > 0$ denote the optimal constant of the Gagliardo-Nirenberg inequality

$$\left(\int_{\mathbb{R}^2} d^2x |\nabla u(x)|^2 \right) \left(\int_{\mathbb{R}^2} d^2y |u(y)|^2 \right) \geq \frac{a^*}{2} \left(\int_{\mathbb{R}^2} d^2x |u(x)|^4 \right).$$

It is then easy to prove that $\int_{\mathbb{R}^2} d^2x |W^-(x)| < a^*$ implies Condition (5.5). On the other hand, (5.5) implies $a > -a^*$. While (5.5) is in general a weaker condition than $\int_{\mathbb{R}^2} d^2x |W^-(x)| < a^*$, for $W \leq 0$, they are equivalent. Consequently, for nonpositive W and for $a < -a^*$, the nonlinear Hartree functional is not bounded from below in the limit $N \rightarrow \infty$, which in particular implies that $H_{W_\beta, t}$ is not stable of the second kind. It is also known that a^* is the critical threshold for blow-up solutions, that is, for $a \leq -a^*$ the solution of (5.3) may blow up in finite time [10, 11, 12, 29, 69, 71].

The condition $H_{W_\beta, t} \geq -CN$ is needed in our proof to control the kinetic energy of those particles which leave the condensate, see Lemma 5.3.8. In prior works, it was necessary to control the quantity $\|\nabla_1 q_1 \Psi_t\|$ sufficiently well in order to show convergence of the reduced density matrices, using the method of counting as introduced in [61]. While it is possible to

obtain an a priori estimate of $\|\nabla_1 q_1 \Psi_t\|$ for repulsive interactions, it is not obvious how one could generalize this estimate for nonpositive W . Our strategy to overcome this difficulty is to control the quantity $\|q_2 \nabla_1 \Psi_t\|$ instead. Under some natural assumptions (see (A2), (A4) and (A5) below), it is possible to obtain a sufficient bound of $\|q_2 \nabla_1 \Psi_t\|$, if initially the variance of the energy

$$\text{Var}_{H_{W_\beta,0}}(\Psi_0) = \frac{1}{N^2} \langle\langle \Psi_0, (H_{W_\beta,0} - \langle\langle \Psi_0, H_{W_\beta,0} \Psi_0 \rangle\rangle)^2 \Psi_0 \rangle\rangle \quad (5.7)$$

is small and $H_{W_\beta,t}$ is stable of second kind. For product states $\Psi_0 = \varphi^{\otimes k}$, with φ regular enough, a straightforward calculation yields $\text{Var}_{H_{W_\beta,0}}(\Psi_0) \leq C(1 + N^{-1+\beta} + N^{-2+2\beta})$, see Lemma 5.3.8. Therefore, for $\beta < 1$, there exist initial states Ψ_0 , for which the variance is small. The strategy to control $\|q_2 \nabla_1 \Psi_t\|$ instead of $\|\nabla_1 q_1 \Psi_t\|$ by means of the energy variance was already used in [37] where the derivation of the Maxwell-Schrödinger equations from the Pauli-Fierz Hamiltonian was shown. Adopting this method, we are able to prove convergence of $\gamma_{\Psi_t}^{(1)}$ to $|\varphi_t\rangle\langle\varphi_t|$ in trace norm as $N \rightarrow \infty$ for $0 < \beta < 1$ with convergence rate of order $N^{-\eta}$, $\eta > 0$, if the Assumptions (A1)-(A5) (see below) are fulfilled.

A stronger statement than convergence in trace norm is convergence in Sobolev trace norm. For external potentials $A_t \in L^p(\mathbb{R}^2, \mathbb{R})$, with $p \in]2, \infty]$, we are able to show

$$\lim_{N \rightarrow \infty} \text{Tr} \left| \sqrt{1 - \Delta} (\gamma_{\Psi_t}^{(1)} - |\varphi_t\rangle\langle\varphi_t|) \sqrt{1 - \Delta} \right| = 0, \quad (5.8)$$

if initially the energy per particle $N^{-1} \langle\langle \Psi_0, H_{W_\beta,0} \Psi_0 \rangle\rangle$ is close to the NLS energy $\langle\varphi_0, (-\Delta + \frac{a}{2}|\varphi_0|^2 + A_0) \varphi_0 \rangle$. To obtain this type of convergence, we adapt some recent results of [2, 51], where a similar statement was proven.

The rigorous derivation of effective evolution equations has a long history, see e.g. [2, 4, 5, 7, 8, 9, 14, 17, 18, 19, 20, 25, 26, 30, 31, 32, 34, 49, 50, 51, 53, 54, 55, 59, 60, 61, 65] and references therein. In particular, for the two-dimensional case we consider, it has been proven, for $0 < \beta < 3/4$ and W nonnegative, that $\gamma_{\Psi_t}^{(1)}$ converges to $|\varphi_t\rangle\langle\varphi_t|$ as $N \rightarrow \infty$ [30]. We extend this result to all $\beta > 0$ in Chapter 3. For $A(x) = |x|^2$ and $W \leq 0$ sufficiently small such that $H_{W_\beta,t} \geq -CN$, the respective convergence has been proven in [14] for $0 < \beta < 1/6$. One key estimate of the proof was to show the stability condition $H_{W_\beta,t} \geq -CN$. The authors note that their proof actually works for all $0 < \beta < 3/4$, if $H_{W_\beta,t} \geq -CN$ holds. As mentioned, this was subsequently proven by [47] in a more general setting.

Recently, the validity of the Bogoloubov approximation for the two-dimensional attractive bose gas was shown in [55] for $0 < \beta < 1$. In contrast to our result, the authors were actually able to achieve norm convergence and did not need to impose the stability condition $H_{W_\beta,t} \geq -CN$, but only required the bound $\int_{\mathbb{R}^2} d^2x |W^-(x)| < a^*$. They then use some refined localization method on the number of particles in different excitation sectors. This strategy enables them to analyze the dynamics without any external field. We want to emphasize that norm convergence is a stronger statement than convergence in the topology of reduced densities. However, convergence in Sobolev trace norm as defined in (5.8) does

in general not follow from norm convergence.

For $0 < \beta < 1/4$, it can be verified that the methods presented in [59], where the attractive three dimensional case is treated, can be applied, assuming some regularity conditions on φ_t (the corresponding conditions for the three dimensional system were proven in [16]). Interestingly, this proof does not restrict the strength of the nonpositive potential nor does it require stability of second kind, but rather assumes a sufficiently fast convergence of $\gamma_{\Psi_0}^{(1)}$ to $|\varphi_0\rangle\langle\varphi_0|$. Therefore, one can prove BEC in two dimensions for $\beta < 1/4$ and arbitrary strong attractive interactions for times for which the solution φ_t exists and is regular enough, that is, before some possible blow-up.

5.2 Main result

We will require the following assumptions:

(A1) For $\beta > 0$, let W_β be given by $W_\beta(x) = N^{-1+2\beta}W(N^\beta x)$, for $W \in L_c^\infty(\mathbb{R}^2, \mathbb{R})$, W spherically symmetric. We assume that there exist constants $0 < \epsilon, \mu < 1$ such that

$$H_{W_\beta, t}^{(\epsilon, \mu)} = (1 - \epsilon) \sum_{k=1}^N (-\Delta_k) + \sum_{i < j} W_\beta(x_i - x_j) + (1 - \mu) \sum_{k=1}^N A_t(x_k) \geq -CN.$$

(A2) For any real-valued function f , decompose $f(x) = f^+(x) - f^-(x)$ with $f^+(x), f^-(x) \geq 0$, such that the supports of f^+ and f^- are disjoint. We assume that $A_t^- \in L^\infty(\mathbb{R}^2, \mathbb{R})$. Furthermore, we assume that A_t is differentiable with respect to t and fulfills

$$\dot{A}_t \in C(\mathbb{R}, L^\infty(\mathbb{R}^2, \mathbb{R})), \nabla \dot{A}_t \in C(\mathbb{R}, L^\infty(\mathbb{R}^2, \mathbb{R})), \Delta \dot{A}_t \in C(\mathbb{R}, L^\infty(\mathbb{R}^2, \mathbb{R})).$$

(A3) For any $s \in \mathbb{R}$, we denote for $k \in \mathbb{N}$ the domain of the self-adjoint operator $(H_{W_\beta, s})^k$ by $\mathcal{D}((H_{W_\beta, s})^k)$. Define the energy variance $\text{Var}_{H_{W_\beta, s}} : \mathcal{D}((H_{W_\beta, s})^2) \rightarrow \mathbb{R}^+$ as

$$\text{Var}_{H_{W_\beta, s}}(\Psi) = \frac{1}{N^2} \langle\langle \Psi, (H_{W_\beta, s} - \langle\langle \Psi, H_{W_\beta, s} \Psi \rangle\rangle)^2 \Psi \rangle\rangle.$$

We then require $\text{Var}_{H_{W_\beta, 0}}(\Psi_0) \leq CN^{-\delta}$ for some $\delta > 0$.

(A4) Let φ_t the solution to $i\partial_t \varphi_t = h_{a, t}^{\text{NLS}} \varphi_t$, $\|\varphi_0\| = 1$. We assume that $\varphi_t \in H^4(\mathbb{R}^2, \mathbb{C})$.

(A5) Assume that the energy per particle

$$N^{-1} |\langle\langle \Psi_0, H_{W_\beta, 0} \Psi_0 \rangle\rangle| \leq C$$

and the NLS energy

$$\left| \langle \varphi_0, \left(-\Delta + \frac{a}{2} |\varphi_0|^2 + A_0 \right) \varphi_0 \rangle \right| \leq C$$

are bounded uniformly in N initially.

(A5)' Assume that there exists a $\delta > 0$, such that

$$\left| N^{-1} \langle\langle \Psi_0, H_{W_\beta,0} \Psi_0 \rangle\rangle - \langle \varphi_0, \left(-\Delta + \frac{a}{2} |\varphi_0|^2 + A_0 \right) \varphi_0 \rangle \right| \leq CN^{-\delta}.$$

Remark 5.2.1 (a) Note that (A1) together with (A2) directly implies $H_{W_\beta,t}^{(\epsilon,0)} \geq -CN$, $H_{W_\beta,t}^{(0,\mu)} \geq -CN$ and $H_{W_\beta,t} = H_{W_\beta,t}^{(0,0)} \geq -CN$. As mentioned in the introduction, (A1) and (A2) are fulfilled for $A(x) \geq C|x|^s$, $s > 0$ for any $0 < \beta < \frac{s+1}{s+2}$, assuming (5.5). [47].

- (b) Assuming $\Psi_0 = \varphi_0^{\otimes N}$ with $\varphi_0 \in W^{2,\infty}(\mathbb{R}^2, \mathbb{C}) \cap H^1(\mathbb{R}^2, \mathbb{C})$, $\|\varphi_0\| = 1$ such that $\langle \varphi_0, A_0 \varphi_0 \rangle + \langle \varphi_0, A_0^2 \varphi_0 \rangle \leq C$, it follows that $\text{Var}_{H_{W_\beta,0}}(\Psi_0) \leq C(N^{-1+\beta} + N^{-2+2\beta})$, see Lemma 5.5.1; and hence (A3) is then valid for all $0 < \beta < 1$.
- (c) For $A_t \in \{0, |x|^2\}$, (A4) follows from the persistence of regularity of solutions, assuming $\varphi_0 \in H^4(\mathbb{R}^2, \mathbb{C})$, $\|A_0^2 \varphi_0\| < \infty$, see Appendix 5.5.2. However, for regular enough external potentials, $a > -a^*$ and regular enough φ_0 we believe (A4) to be valid, too.
- (d) It is interesting to note that both (A1) and (A3) can be fulfilled for $0 < \beta < 1$, while it is unclear if they hold for $\beta \geq 1$.

We now state our main Theorem:

Theorem 5.2.2 Let $\Psi_0 \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap \mathcal{D}((H_{W_\beta,0})^2)$ with $\|\Psi_0\| = 1$. Let $\varphi_0 \in L^2(\mathbb{R}^2, \mathbb{C})$ with $\|\varphi_0\| = 1$ and assume $\lim_{N \rightarrow \infty} \left(N^\delta \text{Tr}[\gamma_{\Psi_0}^{(1)} - |\varphi_0\rangle\langle\varphi_0|] \right) = 0$ for some $\delta > 0$. Let Ψ_t the unique solution to $i\partial_t \Psi_t = H_{W_\beta,t} \Psi_t$ with initial datum Ψ_0 . Let φ_t the unique solution to $i\partial_t \varphi_t = h_{a,t}^{\text{NLS}} \varphi_t$ with initial datum φ_0 .

- (a) (Convergence in trace norm) Assume (A1)-(A5). Then, for any $t > 0$

$$\lim_{N \rightarrow \infty} \gamma_{\Psi_t}^{(1)} = |\varphi_t\rangle\langle\varphi_t| \quad (5.9)$$

in trace norm.

- (b) (Convergence in Sobolev trace norm) Assume (A1)-(A5) and (A5)'. Furthermore, assume that $A_t \in L^p(\mathbb{R}^2, \mathbb{R})$ holds for some $p \in]2, \infty]$ and for all $t \in \mathbb{R}$. Then, for any $t > 0$

$$\lim_{N \rightarrow \infty} \text{Tr} \left| \sqrt{1 - \Delta} (\gamma_{\Psi_t}^{(1)} - |\varphi_t\rangle\langle\varphi_t|) \sqrt{1 - \Delta} \right| = 0. \quad (5.10)$$

Remark 5.2.3 (a) In our proof we will give explicit error estimates in terms of the particle number N . We shall show that the rate of convergence is of order $N^{-\delta}$ for some $\delta > 0$. See (5.21) for the precise error estimate.

(b) Under assumption (A2), the domains $\mathcal{D}(H_{W_\beta,t})$ and $\mathcal{D}((H_{W_\beta,t})^2)$ of the time-dependent Hamiltonian $H_{W_\beta,t}$ are time-invariant, see Appendix 5.5.3. Therefore, the condition $\Psi_0 \in \mathcal{D}((H_{W_\beta,0})^2)$ is sufficient to define and to differentiate the variance of the energy $\text{Var}_{H_{W_\beta,t}}(\Psi_t)$.

(c) For $A_t(x) = |x|^2$, $0 < \beta < 3/4$ and under condition (5.5), the assumptions (A1)-(A5) can be fulfilled by choosing $\Psi_0 = \varphi_0^{\otimes N}$ with φ_0 regular enough. We are therefore able to reproduce the result presented in [14] under slightly different assumptions, using the result of [47] which implies (A1).

(d) For external potentials A_t which are bounded from below, assumption (A1) has been proven for all $0 < \beta \leq 1/2$, under the condition (5.5) [45]. We are therefore able to control the convergence of $\gamma_{\Psi_t}^{(1)}$ to $|\varphi_t\rangle\langle\varphi_t|$ in Sobolev trace norm as $N \rightarrow \infty$ for $0 < \beta \leq 1/2$.

(e) In our estimates, we need the regularity conditions

$$\|\Delta\varphi_t\|_\infty < \infty, \|\nabla\varphi_t\|_\infty < \infty, \|\varphi_t\|_\infty < \infty, \|\nabla\varphi_t\| < \infty, \|\Delta\varphi_t\| < \infty.$$

That is, we need $\varphi_t \in H^2(\mathbb{R}^2, \mathbb{C}) \cap W^{2,\infty}(\mathbb{R}^2, \mathbb{C})$. Then, $\|\Delta|\varphi_t|^2\|$ which also appears in our estimates, can be bounded by

$$\begin{aligned} \Delta|\varphi_t|^2 &= \varphi_t^* \Delta \varphi_t + \varphi_t \Delta \varphi_t^* + 2(\nabla \varphi_t^*) \cdot (\nabla \varphi_t) \\ \|\Delta|\varphi_t|^2\| &\leq 2\|\Delta\varphi_t\| \|\varphi_t\|_\infty + 2\|\nabla\varphi_t\| \|\nabla\varphi_t\|_\infty \end{aligned}$$

Recall the Sobolev embedding Theorem, which implies in particular $H^k(\mathbb{R}^2, \mathbb{C}) = W^{k,2}(\mathbb{R}^2, \mathbb{C}) \subset C^{k-2}(\mathbb{R}^2, \mathbb{C})$. If $\varphi \in C^2(\mathbb{R}^2, \mathbb{C}) \cap H^2(\mathbb{R}^2, \mathbb{C})$, then $\varphi \in W^{2,\infty}(\mathbb{R}^2, \mathbb{C})$ follows since both φ and $\nabla\varphi$ have to decay at infinity. Thus, $\varphi_t \in H^4(\mathbb{R}^2, \mathbb{C})$ implies $\varphi_t \in H^2(\mathbb{R}^2, \mathbb{C}) \cap W^{2,\infty}(\mathbb{R}^2, \mathbb{C})$, which suffices for our estimates¹.

5.3 Proof of Theorem 5.2.2 (a)

Notation 5.3.1 We will denote by $\mathcal{K}(\varphi_t, A_t)$ a constant depending on time, via $\|\dot{A}_t\|_\infty$, $\|A_t^-\|_\infty$, $\int_0^t ds \|\dot{A}_s\|_\infty$ and $\|\varphi_t\|_{H^4}$. As mentioned above, we make use of the embedding $H^2(\mathbb{R}^2, \mathbb{C}) \cap W^{2,\infty}(\mathbb{R}^2, \mathbb{C}) \subseteq H^4(\mathbb{R}^2, \mathbb{C})$.

Next, we will define a convenient functional for proving the Theorem 5.2.2.

Definition 5.3.2 Let $\Psi \in L^2(\mathbb{R}^{2N}, \mathbb{C}) \cap \mathcal{D}((H_{W_\beta,0})^2)$ and let $\varphi \in L^2(\mathbb{R}^2, \mathbb{C})$, $\|\varphi\| = 1$. Define

$$\begin{aligned} \alpha : L^2(\mathbb{R}^{2N}, \mathbb{C}) \times L^2(\mathbb{R}^2, \mathbb{C}) &\rightarrow \mathbb{R}^+, \\ \alpha(\Psi, \varphi) &= \langle\langle \Psi, q_1^\varphi \Psi \rangle\rangle + \text{Var}_{H_{W_\beta,0}}(\Psi). \end{aligned} \tag{5.11}$$

¹ Actually, $\varphi_t \in H^{3+\epsilon}(\mathbb{R}^2, \mathbb{C})$ for some $\epsilon > 0$ would suffice for our estimates. Note that it is reasonable to expect persistence of regularity of φ_t assuming $\varphi_t \in L^\infty(\mathbb{R}^2, \mathbb{C})$, see also Appendix 5.5.2.

Using a general strategy, we will estimate the time derivative $\frac{d}{dt}\alpha(\Psi_t, \varphi_t)$. In particular, we show that

$$\frac{d}{dt}\alpha(\Psi_t, \varphi_t) \leq \mathcal{K}(\varphi_t, A_t) (\alpha(\Psi_t, \varphi_t) + N^{-\delta})$$

holds for some $\delta > 0$. By a Grönwall estimate, which precise form can be found below, we then obtain $\alpha_t(\Psi_t, \varphi_t) \rightarrow 0$ as $N \rightarrow \infty$, if $\alpha(\Psi_0, \varphi_0)$ converges to zero.

Lemma 5.3.3 *Let $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap \mathcal{D}((H_{W_\beta, \cdot})^2)$, $\|\Psi\| = 1$ and let $\varphi \in L^2(\mathbb{R}^2, \mathbb{C})$, $\|\varphi\| = 1$. Let $\alpha(\Psi, \varphi)$ be defined as above. Then,*

$$\begin{aligned} \lim_{N \rightarrow \infty} \alpha(\Psi, \varphi) = 0 &\Leftrightarrow \lim_{N \rightarrow \infty} \gamma_\Psi^{(1)} = |\varphi\rangle\langle\varphi| \text{ in trace norm} \\ \text{and } \lim_{N \rightarrow \infty} \text{Var}_{H_{W_\beta, \cdot}}(\Psi) &= 0. \end{aligned} \quad (5.12)$$

Proof: $\lim_{N \rightarrow \infty} \langle\langle \Psi, q_1^\varphi \Psi \rangle\rangle = 0 \Leftrightarrow \lim_{N \rightarrow \infty} \gamma_\Psi^{(1)} = |\varphi\rangle\langle\varphi|$ in trace norm follows from Lemma 2.0.11. \square

Definition 5.3.4 *Let*

$$Z_\beta^\varphi(x_j, x_k) = W_\beta(x_j - x_k) - \frac{a}{N-1} |\varphi|^2(x_j) - \frac{a}{N-1} |\varphi|^2(x_k). \quad (5.13)$$

Define the functional $\gamma : L^2(\mathbb{R}^{2N}, \mathbb{C}) \times L^2(\mathbb{R}^2, \mathbb{C}) \rightarrow \mathbb{R}_0^+$ by

$$\gamma(\Psi, \varphi) = 2N |\langle\langle \Psi, p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 p_2 \Psi \rangle\rangle| \quad (5.14)$$

$$+ 2N |\langle\langle \Psi, p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 q_2 \Psi \rangle\rangle| \quad (5.15)$$

$$+ 2N |\langle\langle \Psi, q_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 q_2 \Psi \rangle\rangle|. \quad (5.16)$$

Lemma 5.3.5 *Let Ψ_t the unique solution to $i\partial_t \Psi_t = H_{W_\beta, t} \Psi_t$ with initial datum $\Psi_0 \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap \mathcal{D}((H_{W_\beta, 0})^2)$, $\|\Psi_0\| = 1$. Let φ_t the unique solution to $i\partial_t \varphi_t = h_{a,t}^{NLS} \varphi_t$ with initial datum $\varphi_0 \in H^2(\mathbb{R}^2, \mathbb{C})$, $\|\varphi_0\| = 1$. Let $\alpha(\Psi_t, \varphi_t)$ be defined as in Definition 5.3.2. Then*

$$\frac{d}{dt} \alpha(\Psi_t, \varphi_t) \leq \gamma(\Psi_t, \varphi_t) + \left| \frac{d}{dt} \text{Var}_{H_{W_\beta, t}}(\Psi_t) \right|. \quad (5.17)$$

Remark 5.3.6 *The three different contributions of $\gamma(\Psi, \varphi)$ can be identified with three distinct transitions of particles out of the condensate described by φ . The first line can be identified as the interaction of two particles in the state φ , causing one particle to leave the condensate. The second line estimates the evaporation of two particles. The last contribution describes the interaction of one particle in the condensate with one particle outside the condensate, causing the particle in the state φ to leave the condensate.*

Proof: For the proof of the Lemma we restore the upper index φ_t in order to pay respect to the time dependence of $p_1^{\varphi_t}$ and $q_1^{\varphi_t}$. The proof is a straightforward calculation of

$$\begin{aligned} & \frac{d}{dt} \langle\langle \Psi_t, q_1^{\varphi_t} \Psi_t \rangle\rangle \\ &= i \langle\langle H_{W_\beta, t} \Psi_t, q_1^{\varphi_t} \Psi_t \rangle\rangle - i \langle\langle \Psi_t, q_1^{\varphi_t} H_{W_\beta, t} \Psi_t \rangle\rangle - i \langle\langle \Psi_t, [-\Delta_1 + a|\varphi_t|^2(x_1) + A_t(x_1), q_1^{\varphi_t}] \Psi_t \rangle\rangle \\ &= i(N-1) \langle\langle \Psi_t, [Z_\beta^{\varphi_t}(x_1, x_2), q_1^{\varphi_t}] \Psi_t \rangle\rangle = -2(N-1) \operatorname{Im} (\langle\langle \Psi_t, Z_\beta^{\varphi_t}(x_1, x_2) q_1^{\varphi_t} \Psi_t \rangle\rangle). \end{aligned}$$

Using the identity $1 = p_1^{\varphi_t} + q_1^{\varphi_t}$, we obtain

$$\begin{aligned} \frac{d}{dt} \langle\langle \Psi_t, q_1^{\varphi_t} \Psi_t \rangle\rangle &= -2(N-1) \operatorname{Im} (\langle\langle \Psi_t, p_1^{\varphi_t} Z_\beta^{\varphi_t}(x_1, x_2) q_1^{\varphi_t} \Psi_t \rangle\rangle) \\ &= -2(N-1) \operatorname{Im} (\langle\langle \Psi_t, p_1^{\varphi_t} p_2^{\varphi_t} Z_\beta^{\varphi_t}(x_1, x_2) q_1^{\varphi_t} p_2^{\varphi_t} \Psi_t \rangle\rangle) \\ &\quad -2(N-1) \operatorname{Im} (\langle\langle \Psi_t, p_1^{\varphi_t} p_2^{\varphi_t} Z_\beta^{\varphi_t}(x_1, x_2) q_1^{\varphi_t} q_2^{\varphi_t} \Psi_t \rangle\rangle) \\ &\quad -2(N-1) \operatorname{Im} (\langle\langle \Psi_t, p_1^{\varphi_t} q_2^{\varphi_t} Z_\beta^{\varphi_t}(x_1, x_2) q_1^{\varphi_t} p_2^{\varphi_t} \Psi_t \rangle\rangle) \\ &\quad -2(N-1) \operatorname{Im} (\langle\langle \Psi_t, p_1^{\varphi_t} q_2^{\varphi_t} Z_\beta^{\varphi_t}(x_1, x_2) q_1^{\varphi_t} q_2^{\varphi_t} \Psi_t \rangle\rangle). \end{aligned}$$

Note that $\operatorname{Im} (\langle\langle \Psi_t, p_1^{\varphi_t} q_2^{\varphi_t} Z_\beta^{\varphi_t}(x_1, x_2) q_1^{\varphi_t} p_2^{\varphi_t} \Psi_t \rangle\rangle) = 0$, which concludes the proof. \square

Lemma 5.3.7 *Let Ψ_t the unique solution to $i\partial_t \Psi_t = H_{W_\beta, t} \Psi_t$ with initial datum $\Psi_0 \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap \mathcal{D}(H_{W_\beta, 0}^2)$, $\|\Psi_0\| = 1$. Let φ_t the unique solution to $i\partial_t \varphi_t = h_{a, t}^{NL} \varphi_t$ with initial datum $\varphi_0 \in L^2(\mathbb{R}^2, \mathbb{C})$, $\|\varphi_0\| = 1$. Assume (A1)-(A5). Then,*

$$\gamma(\Psi_t, \varphi_t) \leq \mathcal{K}(\varphi_t, A_t) \ln(N)^{1/2} (\alpha(\Psi_t, \varphi_t) + N^{-2\beta} \ln(N)^{1/2} + N^{-1/3} \ln(N)^{3/2}), \quad (5.18)$$

$$\left| \frac{d}{dt} \operatorname{Var}_{H_{W_\beta, t}}(\Psi_t) \right| \leq \mathcal{K}(\varphi_t, A_t) (\alpha(\Psi_t, \varphi_t) + N^{-1}). \quad (5.19)$$

The proof of this Lemma can be found in Section 5.3.2.

Proof of Theorem 5.2.2 (a): Once we have proven Lemma 5.3.7, we obtain with Grönwall's Lemma that

$$\begin{aligned} \alpha(\Psi_t, \varphi_t) &\leq N^{\frac{\int_0^t ds \mathcal{K}(\varphi_s, A_s)}{\ln(N)^{1/2}}} \alpha(\Psi_0, \varphi_0) \\ &\quad + \int_0^t ds \mathcal{K}(\varphi_s, A_s) N^{\frac{\int_s^t d\tau \mathcal{K}(\varphi_\tau, A_\tau)}{\ln(N)^{1/2}}} (N^{-2\beta} \ln(N) + N^{-1/3} \ln(N)^2). \end{aligned} \quad (5.20)$$

Note that under the assumptions (A2) and (A4) there exists a time-dependent constant $C_t < \infty$, such that $\int_0^t ds \mathcal{K}(\varphi_s, A_s) \leq C_t$. Furthermore, the assumption

$$\lim_{N \rightarrow \infty} \left(N^\delta \operatorname{Tr} |\gamma_{\Psi_0}^{(1)} - |\varphi_0\rangle\langle\varphi_0|| \right) = 0$$

for some $\delta > 0$ then implies together with (A3)

$$\lim_{N \rightarrow \infty} \left(N^{\frac{\int_0^t ds \mathcal{K}(\varphi_s, A_s)}{\ln(N)^{1/2}}} \alpha(\Psi_0, \varphi_0) \right) = 0,$$

since $\langle\langle \Psi, q_1^\varphi \Psi \rangle\rangle \leq \text{Tr}|\gamma_\Psi^{(1)} - |\varphi\rangle\langle\varphi|| \leq \sqrt{8\langle\langle \Psi, q_1^\varphi \Psi \rangle\rangle}$, see [34]. Therefore,

$$\begin{aligned} \text{Tr}|\gamma_{\Psi_t}^{(1)} - |\varphi_t\rangle\langle\varphi_t|| &\leq C N^{\frac{C_t}{2\ln(N)^{1/2}} - \delta/2} \\ &+ \sqrt{C_t N^{\frac{\sup_{s \in [0, t]} |C_t - C_s|}{\ln(N)^{1/2}}} (N^{-2\beta} \ln(N) + N^{-1/3} \ln(N)^2)}. \end{aligned} \quad (5.21)$$

This proves Theorem 5.2.2 (a). \square

5.3.1 Energy estimates

Lemma 5.3.8 *Let $\Psi_0 \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap \mathcal{D}((H_{W_\beta, 0})^2)$ with $\|\Psi_0\| = 1$. Let Ψ_t the unique solution to $i\partial_t \Psi_t = H_{W_\beta, 0} \Psi_t$ with initial datum Ψ_0 , $\|\Psi_0\| = 1$. Let φ_t the unique solution to $i\partial_t \varphi_t = h_{a,t}^{NLS} \varphi_t$ with initial datum $\varphi_0 \in L^2(\mathbb{R}^2, \mathbb{C})$, $\|\varphi_0\| = 1$. Assume (A1), (A2), (A4) and (A5). Then,*

(a)

$$\|\nabla_1 \Psi_t\| \leq \mathcal{K}(\varphi_t, A_t). \quad (5.22)$$

(b)

$$\|q_2^{\varphi_t} \nabla_1 \Psi_t\|^2 \leq \mathcal{K}(\varphi_t, A_t) (\alpha(\Psi_t, \varphi_t) + N^{-1/2}). \quad (5.23)$$

(c) For any $p \in \mathbb{N}$, there exists a constant C_p , depending on p , such that

$$\left\| \sqrt{|NW_\beta(x_1 - x_2)|} q_1^{\varphi_t} q_2^{\varphi_t} \Psi_t \right\|^2 \leq \mathcal{K}(\varphi_t, A_t) C_p N^{\beta/p} (\alpha(\Psi_t, \varphi_t) + N^{-1/2}). \quad (5.24)$$

Proof:

(a) Using Assumption (A1) together with (A2), we directly obtain the operator inequality

$$-\sum_{k=1}^N \epsilon \Delta_k \leq H_{W_\beta, t} + CN.$$

Using $\frac{d}{dt} N^{-1} \langle\langle \Psi_t, H_{W_\beta, t} \Psi_t \rangle\rangle \leq \|\dot{A}_t\|_\infty$ together with (A5), the energy per particle $N^{-1} \langle\langle \Psi_t, H_{W_\beta, t} \Psi_t \rangle\rangle \leq \mathcal{K}(\varphi_t, A_t)$ is uniformly bounded in N . Since Ψ_t is symmetric, we obtain

$$N\epsilon \langle\langle \Psi_t, -\Delta_1 \Psi_t \rangle\rangle = \langle\langle \Psi_t, \left(-\sum_{k=1}^N \epsilon \Delta_k \right) \Psi_t \rangle\rangle \leq \mathcal{K}(\varphi_t, A_t) N.$$

(b) (see also [37] for a similar estimate.) We estimate

$$\begin{aligned}
\epsilon \|q_2 \nabla_1 \Psi_t\|^2 &= \frac{1}{N-1} \langle\langle \Psi_t, q_2 \epsilon \sum_{k=1}^N (-\Delta_k) q_2 \Psi_t \rangle\rangle - \frac{\epsilon}{N-1} \langle\langle \Psi_t, q_2 (-\Delta_2) q_2 \Psi_t \rangle\rangle \\
&\leq \frac{1}{N-1} \langle\langle \Psi_t, q_2 H_{W_\beta, t} q_2 \Psi_t \rangle\rangle + C \langle\langle \Psi_t, q_1 \Psi_t \rangle\rangle \\
&= \frac{N}{N-1} \langle\langle \Psi_t, q_2 \left(\frac{H_{W_\beta, t}}{N} - N^{-1} \langle\langle \Psi_t, H_{W_\beta, t} \Psi_t \rangle\rangle \right) \Psi_t \rangle\rangle + \frac{1}{N-1} \langle\langle \Psi_t, H_{W_\beta, t} \Psi_t \rangle\rangle \langle\langle \Psi_t, q_2 \Psi_t \rangle\rangle \\
&\quad - \frac{1}{N-1} \langle\langle \Psi_t, q_2 H_{W_\beta, t} p_2 \Psi_t \rangle\rangle + C \langle\langle \Psi_t, q_1 \Psi_t \rangle\rangle \\
&\leq C \text{Var}_{H_{W_\beta, t}}(\Psi_t) + \frac{1}{N-1} |\langle\langle \Psi_t, q_2 H_{W_\beta, t} p_2 \Psi_t \rangle\rangle| + \mathcal{K}(\varphi_t, A_t) \|q_1 \Psi_t\|^2.
\end{aligned}$$

It remains to estimate

$$\begin{aligned}
&\frac{1}{N-1} |\langle\langle \Psi_t, q_2 H_{W_\beta, t} p_2 \Psi_t \rangle\rangle| \\
&\leq \frac{1}{N-1} |\langle\langle \Psi_t, q_2 (-\Delta_2) p_2 \Psi_t \rangle\rangle| + |\langle\langle \Psi_t, q_2 W_\beta (x_1 - x_2) p_2 \Psi_t \rangle\rangle| + \frac{1}{N-1} |\langle\langle \Psi_t, q_2 A_t (x_1) p_2 \Psi_t \rangle\rangle| \\
&\leq \frac{1}{N-1} (\|\nabla_1 \Psi_t\| \|\nabla \varphi_t\| + \|\nabla \varphi_t\|^2) + \|W_\beta\| \|\varphi_t\|_\infty \|\mathbb{1}_{B_{CN-\beta}(0)}(x_1 - x_2) \Psi_t\| + \|\varphi_t\|_\infty^2 \|W_\beta\|_1 \\
&\quad + \frac{1}{N-1} (\|A_t^-\|_\infty + \|\sqrt{A_t^+} \Psi_t\| \|\sqrt{A_t^+} \varphi_t\| + \langle \varphi_t, A_t \varphi_t \rangle),
\end{aligned}$$

where we used $q_2 = 1 - p_2$ for all three contributions in the last inequality. Recall the two-dimensional Sobolev's inequality, which was introduced in Lemma 3.5.5 and [38], Theorem 8.5. For any $\rho \in H^1(\mathbb{R}^2, \mathbb{C})$ and for any $2 \leq p < \infty$, there exists a constant C_p , depending on p , such that

$$\|\rho\|_p^2 \leq C_p (\|\rho\|^2 + \|\nabla \rho\|^2) \quad (5.25)$$

holds. The constant C_p fulfills $C_p \leq Cp$. We use this inequality in the x_1 variable and obtain together with Hölder's inequality, to obtain

$$\begin{aligned}
&\|\mathbb{1}_{B_{CN-\beta}(0)}(x_1 - x_2) \Psi_t\|^2 \\
&\leq \|\mathbb{1}_{B_{CN-\beta}(0)}\|_{\frac{N}{N-1}} \int d^2 x_2 \dots d^2 x_N \left(\int d^2 x_1 |\Psi_t(x_1, \dots, x_N)|^{2N} \right)^{1/N} \\
&\leq CN^{1-2\beta} \int d^2 x_2 \dots d^2 x_N \left(\int d^2 x_1 |\nabla_1 \Psi_t(x_1, \dots, x_N)|^2 + \int d^2 x_1 |\Psi_t(x_1, \dots, x_N)|^2 \right) \\
&\leq CN^{1-2\beta} (\|\nabla_1 \Psi_t\|^2 + \|\Psi_t\|^2).
\end{aligned}$$

With $\|W_\beta\| = CN^{-1+\beta}$, we obtain together with (a)

$$\|W_\beta\| \|\mathbb{1}_{B_{CN-\beta}(0)}(x_1 - x_2) \Psi_t\| \leq \mathcal{K}(\varphi_t, A_t) N^{-1/2}. \quad (5.26)$$

Next, we show that $\|\sqrt{A_t^+}\Psi_t\|$ and $\|\sqrt{A_t^+}\varphi_t\|$ are uniformly bounded in N . Using the operator inequality (A1) together with (A2) and (A5) directly implies

$$\epsilon \langle \Psi_t, \sum_{k=1}^N A_t^+(x_k) \Psi_t \rangle \leq \langle \Psi_t, H_{W_\beta, t} \Psi_t \rangle + \mathcal{K}(\varphi_t, A_t) N \leq \mathcal{K}(\varphi_t, A_t) N.$$

To control $\langle \varphi_t, A_t^+ \varphi_t \rangle$, let $\Omega_t = \varphi_t^{\otimes N}$. Then

$$\begin{aligned} \epsilon \langle \varphi_t, A_t^+ \varphi_t \rangle &\leq N^{-1} \langle \Omega_t, H_{W_\beta, t} \Omega_t \rangle + \mathcal{K}(\varphi_t, A_t) \\ &= \langle \varphi_t, \left(-\Delta + \frac{a}{2} |\varphi_t|^2 + A_t \right) \varphi_t \rangle + \mathcal{K}(\varphi_t, A_t) \\ &\quad + \langle \varphi_t, \left(\frac{1}{2} (N-1) W_\beta * |\varphi_t|^2 - \frac{a}{2} |\varphi_t|^2 \right) \varphi_t \rangle. \end{aligned}$$

Note that

$$\left| \frac{d}{dt} \langle \varphi_t, \left(-\Delta + \frac{a}{2} |\varphi_t|^2 + A_t \right) \varphi_t \rangle \right| \leq \|\dot{A}_t\|_\infty.$$

which implies together with (A5)

$$\langle \varphi_t, \left(-\Delta + \frac{a}{2} |\varphi_t|^2 + A_t \right) \varphi_t \rangle \leq \mathcal{K}(\varphi_t, A_t).$$

Furthermore, we obtain as in (5.38)

$$\begin{aligned} &|\langle \varphi_t, ((N-1)W_\beta * |\varphi_t|^2 - a|\varphi_t|^2) \varphi_t \rangle| \\ &\leq \|\varphi_t\|_\infty^2 (\|NW_\beta * |\varphi_t|^2 - a|\varphi_t|^2\| + \|W_\beta\|_1 \|\varphi_t\|_\infty^2) \\ &\leq \mathcal{K}(\varphi_t, A_t) (N^{-2\beta} \ln(N) + N^{-1}). \end{aligned}$$

This concludes the proof of (b).

(c) For $1 < p < \infty$, we estimate, using Hölder's- and Sobolev's inequality

$$\begin{aligned} &\left\| \sqrt{|NW_\beta(x_1 - x_2)|} q_1 q_2 \Psi_t \right\|^2 \leq \|NW_\beta\|_\infty \left\| \mathbf{1}_{B_{CN-\beta}(0)}(x_1 - x_2) q_1 q_2 \Psi_t \right\|^2 \\ &\leq CN^{2\beta} \int_{\mathbb{R}^{2N-2}} d^2 x_2 \dots d^2 x_N \int_{\mathbb{R}^2} d^2 x_1 |(q_1 q_2 \Psi_t)(x_1, \dots, x_N)|^2 \mathbf{1}_{B_{CN-\beta}(0)}(x_1 - x_2) \\ &\leq C_p N^{2\beta} \left\| \mathbf{1}_{B_{CN-\beta}(0)} \right\|_{\frac{p}{p-1}} \int_{\mathbb{R}^{2N-2}} d^2 x_2 \dots d^2 x_N \left(\int_{\mathbb{R}^2} d^2 x_1 |(q_1 q_2 \Psi_t)(x_1, \dots, x_N)|^{2p} \right)^{1/p} \\ &\leq C_p N^{2\beta(1-\frac{p-1}{p})} \int_{\mathbb{R}^{2N-2}} d^2 x_2 \dots d^2 x_N \left(\int_{\mathbb{R}^2} d^2 x_1 |(\nabla_1 q_1 q_2 \Psi_t)(x_1, \dots, x_N)|^2 \right)^{\frac{p-1}{p}} \\ &\quad \times \left(\int_{\mathbb{R}^2} d^2 \tilde{x}_1 |(q_1 q_2 \Psi_t)(\tilde{x}_1, \dots, x_N)|^2 \right)^{1/p} \end{aligned} \tag{5.27}$$

We use Hölder's inequality with respect to the x_2, \dots, x_N -integration with the conjugate pair $r = \frac{p}{p-1}$ and $s = p$ to obtain

$$(5.27) \leq C_p N^{\frac{2\beta}{p}} \|\nabla_1 q_1 q_2 \Psi_t\|^{2\frac{p-1}{p}} \|q_1 q_2 \Psi_t\|^{\frac{2}{p}}.$$

Note that

$$\|\nabla_1 q_1 q_2 \Psi_t\|^2 \leq 2\|\nabla_1 p_1 q_2 \Psi_t\|^2 + 2\|\nabla_1 q_2 \Psi_t\|^2 \leq \mathcal{K}(\varphi_t, A_t) (\alpha(\Psi_t, \varphi_t) + N^{-1/2}).$$

Renaming p , we thus obtain with part (b), that there exists a constant depending on p such that

$$\left\| \sqrt{|NW_\beta(x_1 - x_2)|} q_1 q_2 \Psi_t \right\|^2 \leq C_p \mathcal{K}(\varphi_t, A_t) N^{\beta/p} (\alpha(\Psi_t, \varphi_t) + N^{-1/2}).$$

□

5.3.2 Proof of Lemma 5.3.7

For the convenience of the reader, we will restate Lemma 3.5.3 in the following.

Definition 5.3.9 For any $0 \leq \beta_1 \leq \beta$, we define

$$U_{\beta_1}(x) = \begin{cases} \frac{a}{\pi} N^{-1+2\beta_1} & \text{for } |x| < N^{-\beta_1}, \\ 0 & \text{else.} \end{cases} \quad (5.28)$$

and

$$h_{\beta_1, \beta}(x) = \frac{1}{2\pi} \int_{\mathbb{R}^2} \ln|x - y| (W_\beta(y) - U_{\beta_1}(y)) d^2y. \quad (5.29)$$

Lemma 5.3.10 For any $0 \leq \beta_1 \leq \beta$, we obtain with the above definition

(a)

$$\Delta h_{\beta_1, \beta} = W_\beta - U_{\beta_1}. \quad (5.30)$$

(b)

$$\|h_{\beta_1, \beta}\| \leq C N^{-1-\beta_1} \ln(N) \text{ for } \beta_1 > 0, \quad (5.31)$$

$$\|h_{0, \beta}\| \leq C N^{-1} \text{ for } \beta > 0, \quad (5.32)$$

$$\|\nabla h_{\beta_1, \beta}\| \leq C N^{-1} (\ln(N))^{1/2}. \quad (5.33)$$

Proof: See the proof of Lemma 3.5.3.

□

We now prove Lemma 5.3.7.

Lemma 5.3.11 *Let $\Psi \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap \mathcal{D}(H_{W_\beta, \cdot})$, $\|\Psi\| = 1$ and let $\varphi \in L^2(\mathbb{R}^2, \mathbb{C})$, $\|\varphi\| = 1$. Assume (A1), (A2) and (A5). Then,*

(a)

$$N |\langle\langle \Psi, p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 p_2 \Psi \rangle\rangle| \leq \mathcal{K}(\varphi, A.) (N^{-1} + N^{-2\beta} \ln(N)). \quad (5.34)$$

(b)

$$N |\langle\langle \Psi, p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 q_2 \Psi \rangle\rangle| \leq \mathcal{K}(\varphi, A.) (\langle\langle \Psi, q_1 \Psi \rangle\rangle + N^{-1/3} \ln(N)^2). \quad (5.35)$$

(c)

$$N |\langle\langle \Psi, q_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 q_2 \Psi \rangle\rangle| \leq \mathcal{K}(\varphi, A.) \ln(N)^{1/2} (\alpha(\Psi, \varphi) + N^{-1/2}). \quad (5.36)$$

(d) Let φ_t the solution to $i\partial_t \varphi_t = h_{a,t}^{NLS} \varphi_t$, $\|\varphi_0\| = 1$. Let Ψ_t the solution to $i\partial \Psi_t = H_{W_\beta, t} \Psi_t$ with $\Psi_0 \in L_s^2(\mathbb{R}^{2N}, \mathbb{C}) \cap \mathcal{D}((H_{W_\beta, 0})^2)$, $\|\Psi_0\| = 1$. Then,

$$\left| \frac{d}{dt} \text{Var}_{H_{W_\beta, t}}(\Psi_t) \right| \leq \mathcal{K}(\varphi_t, A_t) (\alpha(\Psi_t, \varphi_t) + N^{-1}). \quad (5.37)$$

Remark 5.3.12 (a) and (b) have essentially been proven in Chapter 3 for a slightly different definition of $\alpha(\Psi, \varphi)$. It is (c) where the estimates given in Chapter 3 fails. Recall, that we relied on the energy estimates presented in Section 3.5.6 in order to bound the analogous contribution of (c) as presented in Lemma 3.5.7. To prove the energy estimates, it was crucial in Equation (3.109) that $-(1-\epsilon)\Delta_1 + \frac{1}{2}W(x_1 - x_2) \geq 0$ holds as an operator inequality for some $\epsilon > 0$. This forces $\int_{\mathbb{R}^2} W(x) d^2x$ to be nonnegative. In this chapter, we make use of a strategy which was developed in [37] to derive the Maxwell-Schrödinger equations from the Pauli-Fierz Hamiltonian. Instead of estimating $\|\nabla_1 q_1 \Psi\|$, we control $\|\nabla_1 q_2 \Psi\|$ instead, see Lemma 5.3.8.

Proof:

(a) We estimate

$$N |\langle\langle \Psi, p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 p_2 \Psi \rangle\rangle| \leq N \|p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 p_2\|_{\text{op}}.$$

$\|p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 p_2\|_{\text{op}}$ can be estimated using $p_1 q_1 = 0$ and (2.7).

$$\begin{aligned} & N \left\| p_1 p_2 \left(W_\beta(x_1 - x_2) - \frac{a}{N-1} |\varphi(x_1)|^2 - \frac{a}{N-1} |\varphi(x_2)|^2 \right) q_1 p_2 \right\|_{\text{op}} \\ & \leq \|p_1 p_2 (N W_\beta(x_1 - x_2) - a |\varphi(x_1)|^2) p_2\|_{\text{op}} + C \|\varphi\|_\infty^2 N^{-1} \\ & \leq \|\varphi\|_\infty \|N (W_\beta \star |\varphi|^2) - a |\varphi|^2\| + C \|\varphi\|_\infty^2 N^{-1}. \end{aligned}$$

Let h be given by

$$h(x) = \frac{1}{2\pi} \int_{\mathbb{R}^2} d^2y \ln|x-y| NW_\beta(y) - \frac{a}{2\pi} \ln|x|.$$

It then follows

$$\Delta h(x) = NW_\beta(x) - a\delta(x)$$

in the sense of distributions. Since $a = \int_{\mathbb{R}^2} d^2x W(x)$, this implies (see Lemma 5.3.10), $h(x) = 0$ for $x \notin B_{RN^{-\beta}}(0)$, where $RN^{-\beta}$ is the radius of the support of W_β . Thus,

$$\begin{aligned} \|h\|_1 &\leq \frac{1}{2\pi} \int_{\mathbb{R}^2} d^2x \int_{\mathbb{R}^2} d^2y |\ln|x-y|| \mathbb{1}_{B_{RN^{-\beta}}(0)}(x) NW_\beta(y) \\ &\quad + \frac{|a|}{2\pi} \int_{\mathbb{R}^2} d^2x \ln(|x|) \mathbb{1}_{B_{RN^{-\beta}}(0)}(x) \\ &\leq CN^{-2\beta} \ln(N). \end{aligned}$$

Integration by parts and Young's inequality then imply

$$\begin{aligned} \|N(W_\beta \star |\varphi|^2) - a|\varphi|^2\| &= \|(\Delta h) \star |\varphi|^2\| \\ &\leq \|h\|_1 \|\Delta|\varphi|^2\| \leq \mathcal{K}(\varphi, A.) N^{-2\beta} \ln(N). \end{aligned} \tag{5.38}$$

Thus, we obtain the bound

$$N |\langle\langle \Psi, p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 p_2 \widehat{w} \Psi \rangle\rangle| \leq \mathcal{K}(\varphi, A.) (N^{-1} + N^{-2\beta} \ln(N)), \tag{5.39}$$

which then proves (a).

(b) We will first consider the case $0 < \beta \leq 1/3$. Note that $p_1 p_2 Z_\beta^\varphi(x_1, x_2) q_1 q_2 = p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2$. We estimate

$$\begin{aligned} N |\langle\langle \Psi, q_1 q_2 W_\beta(x_1 - x_2) p_1 p_2 \Psi \rangle\rangle| &= \frac{N}{N-1} |\langle\langle q_1 \Psi, \sum_{k=2}^N q_k W_\beta(x_1 - x_k) p_1 p_k \Psi \rangle\rangle| \\ &\leq \frac{N}{N-1} \|q_1 \Psi\| \left\| \sum_{k=2}^N q_k W_\beta(x_1 - x_k) p_1 p_k \Psi \right\| \\ &\leq \langle\langle \Psi, q_1 \Psi \rangle\rangle + \left\| \sum_{k=2}^N q_k W_\beta(x_1 - x_k) p_1 p_k \Psi \right\|^2 \\ &= \langle\langle \Psi, q_1 \Psi \rangle\rangle + (N-1) \|q_2 W_\beta(x_1 - x_2) p_1 p_2 \Psi\|^2 \\ &\quad + (N-1)(N-2) \langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_2 q_3 W_\beta(x_1 - x_3) p_1 p_3 \Psi \rangle\rangle \\ &\leq \langle\langle \Psi, q_1 \Psi \rangle\rangle + N \|W_\beta\|^2 \|\varphi\|_\infty^2 \\ &\quad + N^2 \|p_2 W_\beta(x_1 - x_2) p_1\|_{\text{op}}^2 \|q_1 \Psi\|^2 \\ &\leq \mathcal{K}(\varphi, A.) (\langle\langle \Psi, q_1 \Psi \rangle\rangle + N^{-1+2\beta}). \end{aligned}$$

In the last estimate, we used Lemma 5.3.10 together with Lemma 2.0.5 to estimate $\|p_1 W_\beta(x_1 - x_2) p_2\|_{\text{op}} \leq \|p_1 \sqrt{|W_\beta|}\|_{\text{op}}^2 \leq \|\varphi\|_\infty^2 \|\sqrt{|W_\beta|}\|^2 \leq \mathcal{K}(\varphi, A.) N^{-1}$.

This proves (b) for the case $\beta \leq 1/3$.

(b) for $1/3 < \beta$: We use U_{β_1} from Definition 3.5.2 for some $0 < \beta_1 \leq 1/3$. We then obtain

$$\begin{aligned} & N \langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \Psi \rangle\rangle \\ &= N \langle\langle \Psi, p_1 p_2 U_{\beta_1}(x_1 - x_2) q_1 q_2 \Psi \rangle\rangle \end{aligned} \quad (5.40)$$

$$+ N \langle\langle \Psi, p_1 p_2 (W_\beta(x_1 - x_2) - U_{\beta_1}(x_1 - x_2)) q_1 q_2 \Psi \rangle\rangle. \quad (5.41)$$

Term (5.40) has been controlled above. So we are left to control (5.41).

Let $\Delta h_{\beta_1, \beta} = W_\beta - U_{\beta_1}$, as in Lemma 5.3.10. Integrating by parts and using $\nabla_1 h_{\beta_1, \beta}(x_1 - x_2) = -\nabla_2 h_{\beta_1, \beta}(x_1 - x_2)$ gives

$$\begin{aligned} & N |\langle\langle \Psi, p_1 p_2 (W_\beta(x_1 - x_2) - U_{\beta_1, \beta}(x_1 - x_2)) q_1 q_2 \Psi \rangle\rangle| \\ & \leq N |\langle\langle \nabla_1 p_1 \Psi, p_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) q_1 q_2 \Psi \rangle\rangle| \end{aligned} \quad (5.42)$$

$$+ N |\langle\langle \Psi, p_1 p_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) \nabla_1 q_1 q_2 \Psi \rangle\rangle|. \quad (5.43)$$

Let $t_1 \in \{p_1, \nabla_1 p_1\}$ and let $\Gamma \in \{q_1 \Psi, \nabla_1 q_1 \Psi\}$.

For both (5.42) and (5.43), we use Lemma 2.0.10 with $O_{1,2} = N^{1+\eta/2} q_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) p_2$, $\chi = t_1 \Psi$ and $\Omega = N^{-\eta/2} \Gamma$. This yields

$$(5.42) + (5.43) \leq 2 \sup_{t_1 \in \{p_1, \nabla_1 p_1\}, \Gamma \in \{q_1 \Psi, \nabla_1 q_1 \Psi\}} \left(N^{-\eta} \|\Gamma\|^2 \right) \quad (5.44)$$

$$+ \frac{N^{2+\eta}}{N-1} \|q_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) t_1 p_2 \Psi\|^2 \quad (5.45)$$

$$+ N^{2+\eta} |\langle\langle \Psi, t_1 p_2 q_3 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) \nabla_3 h_{\beta_1, \beta}(x_1 - x_3) t_1 q_2 p_3 \Psi \rangle\rangle|. \quad (5.46)$$

The first term can be bounded using $\|\nabla_1 q_1 \Psi\| \leq \mathcal{K}(\varphi, A.)$.

Using $\|t_1 \Psi\|^2 \leq \mathcal{K}(\varphi, A.)$, we obtain

$$\begin{aligned} (5.45) & \leq \mathcal{K}(\varphi, A.) \frac{N^{2+\eta}}{N-1} \|\nabla_2 h_{\beta_1, \beta}(x_1 - x_2) p_2\|_{\text{op}}^2 \leq \mathcal{K}(\varphi, A.) \frac{N^{2+\eta}}{N-1} \|\varphi\|_\infty^2 \|\nabla h_{\beta_1, \beta}\|^2 \\ & \leq \mathcal{K}(\varphi, A.) N^{\eta-1} \ln(N), \end{aligned}$$

where we used Lemma 5.3.10 in the last step.

Next, we estimate

$$\begin{aligned}
(5.46) &\leq N^{2+\eta} \|p_2 \nabla_2 h_{\beta_1, \beta}(x_1 - x_2) t_1 q_2 \Psi\|^2 \\
&\leq 2N^{2+\eta} \|p_2 h_{\beta_1, \beta}(x_1 - x_2) t_1 \nabla_2 q_2 \Psi\|^2 \\
&\quad + 2N^{2+\eta} \|\langle \varphi(x_2) \rangle \langle \nabla \varphi(x_2) | h_{\beta_1, \beta}(x_1 - x_2) t_1 q_2 \Psi \rangle\|^2 \\
&\leq 2N^{2+\eta} \|p_2 h_{\beta_1, \beta}(x_1 - x_2)\|_{\text{op}}^2 \|t_1 \nabla_2 q_2 \Psi\|^2 \\
&\quad + 2N^{2+\eta} \|\langle \varphi(x_2) \rangle \langle \nabla \varphi(x_2) | h_{\beta_1, \beta}(x_1 - x_2) \rangle\|_{\text{op}}^2 \|t_1 q_2 \Psi\|^2 \\
&\leq \mathcal{K}(\varphi, A.) N^{2+\eta} \|h_{\beta_1, \beta}\|^2 \leq \mathcal{K}(\varphi, A.) N^{\eta-2\beta_1} \ln(N)^2.
\end{aligned}$$

Thus, for all $\eta \in \mathbb{R}$

$$\begin{aligned}
N \langle\langle \Psi, p_1 p_2 (W_\beta(x_1 - x_2) - U_{\beta_1, \beta}(x_1 - x_2)) q_1 q_2 \Psi \rangle\rangle \\
\leq \mathcal{K}(\varphi, A.) (N^{-\eta} + N^{\eta-1} \ln(N) + N^{\eta-2\beta_1} \ln(N)^2).
\end{aligned}$$

Hence, we obtain, using $N^{\eta-1} \ln(N) < N^{\eta-2\beta_1} \ln(N)$,

$$\begin{aligned}
N \langle\langle \Psi, p_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \Psi \rangle\rangle \\
\leq \mathcal{K}(\varphi, A.) \left(\langle\langle \Psi, q_1 \Psi \rangle\rangle + \inf_{\eta > 0} \inf_{\frac{1}{3} \geq \beta_1 > 0} (N^{\eta-2\beta_1} \ln(N)^2 + N^{-1+2\beta_1} + N^{-\eta}) \right).
\end{aligned}$$

and we get (b) in full generality by choosing $\eta = \beta_1 = 1/3$.

(c) First note that

$$N \left| \langle\langle \Psi, q_1 p_2 \frac{a}{N-1} |\varphi(x_1)|^2 q_1 q_2 \Psi \rangle\rangle \right| \leq C \|\varphi\|_\infty^2 \langle\langle \Psi, q_1 \Psi \rangle\rangle.$$

Let U_0 be given as in Lemma 5.3.10. Using Lemma 2.0.5 and integrating by parts we get

$$\begin{aligned}
N |\langle\langle \Psi, q_1 p_2 W_\beta(x_1 - x_2) q_1 q_2 \Psi \rangle\rangle| \\
\leq N |\langle\langle \Psi, q_1 p_2 U_0(x_1 - x_2) q_1 q_2 \Psi \rangle\rangle| + N |\langle\langle \Psi, q_1 p_2 (\Delta_1 h_{0, \beta}(x_1 - x_2)) q_1 q_2 \Psi \rangle\rangle| \\
\leq N \|q_1 \Psi\| \|U_0\|_\infty \|q_1 q_2 \Psi\| \tag{5.47}
\end{aligned}$$

$$+N |\langle\langle \nabla_2 p_2 q_1 \Psi, (\nabla_2 h_{0, \beta}(x_1 - x_2)) q_1 q_2 \Psi \rangle\rangle| \tag{5.48}$$

$$+N |\langle\langle \Psi, q_1 p_2 (\nabla_2 h_{0, \beta}(x_1 - x_2)) \nabla_2 q_1 q_2 \Psi \rangle\rangle|. \tag{5.49}$$

The first contribution is bounded by

$$(5.47) \leq C \langle\langle \Psi, q_1 \Psi \rangle\rangle.$$

The second term (5.48) can be estimated as

$$(5.48) = N |\langle\langle \Delta_2 p_2 q_1 \Psi, h_{0, \beta}(x_1 - x_2) q_1 q_2 \Psi \rangle\rangle| \tag{5.50}$$

$$+N |\langle\langle \nabla_2 p_2 q_1 \Psi, h_{0, \beta}(x_1 - x_2) q_1 \nabla_2 \Psi \rangle\rangle| \tag{5.51}$$

$$+N |\langle\langle \nabla_2 p_2 q_1 \Psi, h_{0, \beta}(x_1 - x_2) q_1 \nabla_2 p_2 \Psi \rangle\rangle|. \tag{5.52}$$

The last contribution (5.49) can be rewritten as

$$(5.49) \leq N |\langle\langle \Psi, q_1 p_2 (\nabla_2 h_{0,\beta}(x_1 - x_2)) \nabla_2 q_1 \Psi \rangle\rangle| \quad (5.53)$$

$$+ N |\langle\langle \Psi, q_1 p_2 (\nabla_2 h_{0,\beta}(x_1 - x_2)) \nabla_2 p_2 q_1 \Psi \rangle\rangle|. \quad (5.54)$$

We estimate each contribution separately, using Lemma 5.3.10 together with Lemma 2.0.5. We obtain

$$(5.50) \leq N \|q_1 \Psi\| \|h_{0,\beta}(x_1 - x_2) \Delta_2 p_2\|_{\text{op}} \|q_1 q_2 \Psi\| \leq C \|\Delta \varphi\|_{\infty} \langle\langle \Psi, q_1 \Psi \rangle\rangle.$$

Analogously,

$$(5.52) \leq N \|q_1 \Psi\| \|h_{0,\beta}(x_1 - x_2) \nabla_2 p_2\|_{\text{op}} \|\nabla \varphi\|_{\infty} \|q_1 \Psi\| \leq C \|\nabla \varphi\|_{\infty}^2 \langle\langle \Psi, q_1 \Psi \rangle\rangle.$$

Next, we control

$$(5.54) \leq N \|q_1 \Psi\| \|p_2 \nabla_2 h_{0,\beta}(x_1 - x_2) \nabla_2 p_2\|_{\text{op}} \|q_1 \Psi\| \leq C \|\nabla \varphi\|_{\infty} \|\varphi\|_{\infty} N \|\nabla h_{0,\beta}\|_1 \|q_1 \Psi\|^2 \leq C \|\nabla \varphi\|_{\infty} \|\varphi\|_{\infty} \langle\langle \Psi, q_1 \Psi \rangle\rangle.$$

To control (5.51) and (5.53), we estimate for $t_2 \in \{p_2, |\varphi(x_2)\rangle \langle (\nabla \varphi)(x_2)|\}$ and $s \in \{h_{0,\beta}, \nabla_2 h_{0,\beta}\}$

$$\begin{aligned} & N |\langle\langle q_1 \Psi, t_2 s (x_1 - x_2) \nabla_2 q_1 \Psi \rangle\rangle| \\ & \leq \ln(N)^{1/2} \|q_1 \Psi\|^2 + \ln(N)^{-1/2} N^2 \|t_2 s (x_1 - x_2)\|_{\text{op}}^2 \|\nabla_2 q_1 \Psi\|^2 \\ & \leq \mathcal{K}(\varphi, A) \ln(N)^{1/2} \left(\text{Var}_{H_{W_{\beta}, \cdot}}(\Psi) + N^{-1/2} + \langle\langle \Psi, q_1 \Psi \rangle\rangle \right). \end{aligned}$$

(d) We estimate

$$\begin{aligned}
\left| \frac{d}{dt} \text{Var}_{H_{W_\beta,t}}(\Psi_t) \right| &= N^{-2} \left| \frac{d}{dt} \langle\langle \Psi_t, (H_{W_\beta,t} - \langle\langle \Psi_t, H_{W_\beta,t} \Psi_t \rangle\rangle)^2 \Psi_t \rangle\rangle \right| \\
&\leq 2N^{-1} \left| \langle\langle \Psi_t, (H_{W_\beta,t} - \langle\langle \Psi_t, H_{W_\beta,t} \Psi_t \rangle\rangle) (\dot{A}_t(x_1) - \langle\langle \Psi_t, \dot{A}_t(x_1) \Psi_t \rangle\rangle) \Psi_t \rangle\rangle \right| \\
&\leq 2N^{-1} \left| \langle\langle \Psi_t, (H_{W_\beta,t} - \langle\langle \Psi_t, H_{W_\beta,t} \Psi_t \rangle\rangle) (p_1 \dot{A}_t(x_1) p_1 - \langle\langle \Psi_t, p_1 \dot{A}_t(x_1) p_1 \Psi_t \rangle\rangle) \Psi_t \rangle\rangle \right| \\
&+ 2N^{-1} \left| \langle\langle \Psi_t, (H_{W_\beta,t} - \langle\langle \Psi_t, H_{W_\beta,t} \Psi_t \rangle\rangle) (p_1 \dot{A}_t(x_1) q_1 - \langle\langle \Psi_t, p_1 \dot{A}_t(x_1) q_1 \Psi_t \rangle\rangle) \Psi_t \rangle\rangle \right| \\
&+ 2N^{-1} \left| \langle\langle \Psi_t, (H_{W_\beta,t} - \langle\langle \Psi_t, H_{W_\beta,t} \Psi_t \rangle\rangle) \left(N^{-1} \sum_{k=1}^N q_k \dot{A}_t(x_k) p_k - \langle\langle \Psi_t, q_1 \dot{A}_t(x_1) p_1 \Psi_t \rangle\rangle \right) \Psi_t \rangle\rangle \right| \\
&+ 2N^{-1} \left| \langle\langle \Psi_t, (H_{W_\beta,t} - \langle\langle \Psi_t, H_{W_\beta,t} \Psi_t \rangle\rangle) (q_1 \dot{A}_t(x_k) q_1 - \langle\langle \Psi_t, q_1 \dot{A}_t(x_k) q_1 \Psi_t \rangle\rangle) \Psi_t \rangle\rangle \right| \\
&\leq 4 \text{Var}_{H_{W_\beta,t}}(\Psi_t) + \left\| (p_1 \dot{A}_t(x_1) p_1 - \langle\langle \Psi_t, p_1 \dot{A}_t(x_1) p_1 \Psi_t \rangle\rangle) \Psi_t \right\|^2 \\
&+ \left\| (p_1 \dot{A}_t(x_1) q_1 - \langle\langle \Psi_t, p_1 \dot{A}_t(x_1) q_1 \Psi_t \rangle\rangle) \Psi_t \right\|^2 \\
&+ \left\| \left(N^{-1} \sum_{k=1}^N q_k \dot{A}_t(x_k) p_k - \langle\langle \Psi_t, q_1 \dot{A}_t(x_1) p_1 \Psi_t \rangle\rangle \right) \Psi_t \right\|^2 \\
&+ \left\| (q_1 \dot{A}_t(x_1) q_1 - \langle\langle \Psi_t, q_1 \dot{A}_t(x_1) q_1 \Psi_t \rangle\rangle) \Psi_t \right\|^2.
\end{aligned}$$

Note that

$$\begin{aligned}
&\left\| (p_1 \dot{A}_t(x_1) p_1 - \langle\langle \Psi_t, p_1 \dot{A}_t(x_1) p_1 \Psi_t \rangle\rangle) \Psi_t \right\|^2 \\
&= \left(\int_{\mathbb{R}^2} d^2 x \dot{A}_t(x) |\varphi_t(x)|^2 \right)^2 \langle\langle \Psi_t, p_1 \Psi_t \rangle\rangle (1 - \langle\langle \Psi_t, p_1 \Psi_t \rangle\rangle) \\
&\leq \mathcal{K}(\varphi_t, A_t) \langle\langle \Psi_t, q_1 \Psi_t \rangle\rangle.
\end{aligned}$$

Furthermore

$$\begin{aligned}
&\left\| \left(N^{-1} \sum_{k=1}^N q_k \dot{A}_t(x_k) p_k - \langle\langle \Psi_t, q_1 \dot{A}_t(x_1) p_1 \Psi_t \rangle\rangle \right) \Psi_t \right\|^2 \\
&= N^{-2} \sum_{k,l=1}^N \langle\langle \Psi_t, p_l \dot{A}_t(x_l) q_l q_k \dot{A}_t(x_k) p_k \Psi_t \rangle\rangle - \left| \langle\langle \Psi_t, q_1 \dot{A}_t(x_1) p_1 \Psi_t \rangle\rangle \right|^2 \\
&\leq \langle\langle \Psi_t, p_1 \dot{A}_t(x_1) q_1 q_2 \dot{A}_t(x_2) p_2 \Psi_t \rangle\rangle + \frac{1}{N} \langle\langle \Psi_t, p_1 \dot{A}_t(x_1) q_1 \dot{A}_t(x_1) p_1 \Psi_t \rangle\rangle + \|\dot{A}_t\|_\infty \langle\langle \Psi_t, q_1 \Psi_t \rangle\rangle \\
&\leq \mathcal{K}(\varphi_t, A_t) \left(\langle\langle \Psi_t, q_1 \Psi_t \rangle\rangle + \frac{1}{N} \right).
\end{aligned}$$

To control the two remaining terms, let $s_1 \in \{p_1, q_1\}$. Then, we need to estimate

$$\begin{aligned} & \left\| \left(s_1 \dot{A}_t(x_1) q_1 - \langle \Psi_t, s_1 \dot{A}_t(x_1) q_1 \Psi_t \rangle \right) \Psi_t \right\|^2 \\ &= \langle \Psi_t, q_1 \dot{A}_t(x_1) s_1 \dot{A}_t(x_1) q_1 \Psi_t \rangle - \left| \langle \Psi_t, s_1 \dot{A}_t(x_1) q_1 \Psi_t \rangle \right|^2 \\ &\leq 2 \|\dot{A}_t\|_\infty^2 \langle \Psi_t, q_1 \Psi_t \rangle. \end{aligned}$$

In total, we obtain

$$\left| \frac{d}{dt} \text{Var}_{H_{W_\beta, t}}(\Psi_t) \right| \leq \mathcal{K}(\varphi_t, A_t) (\alpha(\Psi_t, \varphi_t) + N^{-1}).$$

Combining the estimates (a)-(d), Lemma 5.3.7 is then proven.

□

5.4 Proof of Theorem 5.2.2 (b)

Proof: We make use of the inequality

$$\begin{aligned} \text{Tr} \left| \sqrt{1 - \Delta} (\gamma_{\Psi_t}^{(1)} - |\varphi_t\rangle\langle\varphi_t|) \sqrt{1 - \Delta} \right| &\leq C(1 + \|\nabla_1 \varphi_t\|)^2 \\ &\times (\|q_1 \Psi_t\| + \|q_1 \Psi_t\|^2 + \|\nabla_1 q_1 \Psi_t\| + \|\nabla_1 q_1 \Psi_t\|^2), \end{aligned}$$

which was proven in [51], see also [2]. Using Theorem 5.2.2 (a), we are left to show $\lim_{N \rightarrow \infty} \|\nabla_1 q_1 \Psi_t\| = 0$. In general, this does not follow from $\lim_{N \rightarrow \infty} \|\nabla_1 q_2 \Psi_t\| = 0$. To see this, consider the symmetrized wave-function

$$\Gamma(x_1, \dots, x_N) = \frac{1}{\sqrt{N}} \sum_{k=1}^N \varphi(x_1) \dots \eta(x_k) \dots \varphi(x_N)$$

for $\eta, \varphi \in L^2(\mathbb{R}^2, \mathbb{C})$, $\|\eta\| = \|\varphi\| = 1$, $\langle \eta, \varphi \rangle = 0$. Then

$$\|q_1^\varphi \Gamma\|^2 = N^{-1}, \quad \|\nabla_1 q_2^\varphi \Gamma\|^2 = N^{-1} \|\nabla \varphi\|^2, \quad \|\nabla_1 q_1^\varphi \Gamma\|^2 = N^{-1} \|\nabla \eta\|^2.$$

Note that $\|\nabla \eta\|$ can be chosen arbitrarily. However, for $A_t \in L^p(\mathbb{R}^2, \mathbb{R})$, with $p > 2$, it is possible to control $\|\nabla_1 q_1 \Psi_t\|$ in terms of $\|q_1 \Psi_t\|$, $\|\nabla_1 q_2 \Psi_t\|$ and the energy difference $|N^{-1} \langle \Psi_0, H_{W_\beta, 0} \Psi_0 \rangle - \langle \varphi_0, (-\Delta + \frac{a}{2} |\varphi_0|^2 + A_0) \varphi_0 \rangle|$, assuming Conditions (A2) and (A4). Together with Assumptions (A1), (A3), (A5) and (A5)' and Theorem 5.2.2, part (a), it is

then possible to bound $\|\nabla_1 q_1 \Psi_t\|$ sufficiently well. First, we consider

$$|\|\nabla_1 \Psi_t\|^2 - \|\nabla \varphi_t\|^2| \leq \left| \frac{1}{N} \langle \Psi_0, H_{W_\beta, 0} \Psi_0 \rangle - \langle \varphi_0, \left(-\Delta + \frac{a}{2} |\varphi_0|^2 + A_0 \right) \varphi_0 \rangle \right| \quad (5.55)$$

$$+ \int_0^t ds \left| \langle \Psi_s, \dot{A}_s(x_1) \Psi_s \rangle - \langle \varphi_s, \dot{A}_s \varphi_s \rangle \right| \quad (5.56)$$

$$+ \frac{1}{2} \left| \langle \Psi_t, p_1 p_2 (N-1) W_\beta(x_1 - x_2) p_1 p_2 \Psi_t \rangle - a \langle \varphi_t, |\varphi_t|^2 \varphi_t \rangle \right| \quad (5.57)$$

$$+ N |\langle \Psi_t, p_1 p_2 W_\beta(x_1 - x_2) (1 - p_1 p_2) \Psi_t \rangle| \quad (5.58)$$

$$+ N |\langle \Psi_t, (1 - p_1 p_2) W_\beta(x_1 - x_2) (1 - p_1 p_2) \Psi_t \rangle| \quad (5.59)$$

$$+ |\langle \Psi_t, A_t(x_1) \Psi_t \rangle - \langle \varphi_t, A_t \varphi_t \rangle|. \quad (5.60)$$

We estimate each line separately. From Condition (A5)', it follows that (5.55) $\leq CN^{-\delta}$. Using $\dot{A}_t \in L^\infty(\mathbb{R}^2, \mathbb{R})$, we estimate

$$(5.56) \leq t \sup_{s \in [0, t]} \left(|\langle \varphi_s, \dot{A}_s \varphi_s \rangle| |\langle \Psi_s, q_1^{\varphi_s} \Psi_s \rangle| + 2 \left| \langle \Psi_s, p_1^{\varphi_s} \dot{A}_s(x_1) q_1^{\varphi_s} \Psi_s \rangle \right| + \left| \langle \Psi_s, q_1^{\varphi_s} \dot{A}_s(x_1) q_1^{\varphi_s} \Psi_s \rangle \right| \right)$$

$$\leq t \sup_{s \in [0, t]} \left(\|\dot{A}_s\|_\infty (\|q_1^{\varphi_s} \Psi_s\| + \|q_1^{\varphi_s} \Psi_s\|^2) \right).$$

Next,

$$(5.57) \leq |\langle \varphi_t, (N-1) W_\beta \star |\varphi_t|^2 \varphi_t \rangle| |\langle \Psi_t, p_1 p_2 \Psi_t \rangle| - a \langle \varphi_t, |\varphi_t|^2 \varphi_t \rangle|$$

$$\leq \mathcal{K}(\varphi_t, A_t) \|N W_\beta\|_1 \|q_1 \Psi_t\|^2 + |\langle \varphi_t, ((N-1) W_\beta \star |\varphi_t|^2 - a |\varphi_t|^2) \varphi_t \rangle|$$

$$\leq \mathcal{K}(\varphi_t, A_t) (\langle \Psi_t, q_1 \Psi_t \rangle + N^{-2\beta} \ln(N) + N^{-1}).$$

Note that

$$(5.58) + (5.59) \leq C \left\| \sqrt{N |W_\beta(x_1 - x_2)|} p_1 p_2 \Psi_t \right\|$$

$$\times \left(\left\| \sqrt{N |W_\beta(x_1 - x_2)|} q_1 q_2 \Psi_t \right\| + \left\| \sqrt{N |W_\beta(x_1 - x_2)|} q_1 p_2 \Psi_t \right\| \right)$$

$$+ C \left\| \sqrt{N |W_\beta(x_1 - x_2)|} p_1 q_2 \Psi_t \right\|^2 + C \left\| \sqrt{N |W_\beta(x_1 - x_2)|} q_1 q_2 \Psi_t \right\|^2.$$

Using Lemma 5.3.8, we obtain

$$\left\| \sqrt{N |W_\beta(x_1 - x_2)|} q_1 q_2 \Psi_t \right\|^2 \leq \mathcal{K}(\varphi_t, A_t) C_p N^{\beta/p} (\alpha(\Psi_t, \varphi_t) + N^{-1/2}).$$

Furthermore,

$$\left\| \sqrt{N |W_\beta(x_1 - x_2)|} p_1 \right\|_{\text{op}} \leq \mathcal{K}(\varphi_t, A_t).$$

Note that it was shown in part (a) that $\alpha(\Psi_t, \varphi_t) \leq \mathcal{K}(\varphi_t, A_t)N^{-\delta}$ for some $\delta > 0$. Choosing p large enough, we then obtain $(5.58) + (5.59) \leq \mathcal{K}(\varphi_t, A_t)N^{-\gamma}$, for some $\gamma > 0$. We estimate, using $|\langle\Psi_t, q_1 A_t(x_1) q_1 \Psi_t\rangle| \leq \|q_1 \Psi_t\|(\|A_t \varphi_t\| + \|A_t(x_1) \Psi_t\|)$,

$$\begin{aligned} |(5.60)| &\leq |\langle\varphi_t, A_t \varphi_t\rangle| |\langle\Psi_t, q_1 \Psi_t\rangle| + 2|\langle\Psi_t, p_1 A_t(x_1) q_1 \Psi_t\rangle| + |\langle\Psi_t, q_1 A_t(x_1) q_1 \Psi_t\rangle| \\ &\leq |\langle\varphi_t, A_t \varphi_t\rangle| |\langle\Psi_t, q_1 \Psi_t\rangle| + \|q_1 \Psi_t\|(\|A_t \varphi_t\| + \|A_t(x_1) \Psi_t\|). \end{aligned}$$

If $A_t \in L^\infty(\mathbb{R}^2, \mathbb{R})$ holds, we obtain

$$|(5.60)| \leq \mathcal{K}(\varphi_t, A_t)(\|q_1 \Psi_t\| + \|q_1 \Psi_t\|^2).$$

On the other hand, using Sobolev and Hölder inequality (see the proof of Lemma 5.3.8), together with $|\langle\varphi_t, A_t \varphi_t\rangle| + \|\nabla_1 \Psi_t\| + \|\nabla \varphi_t\| \leq \mathcal{K}(\varphi_t, A_t)$, we obtain, for any $1 < p < \infty$

$$|(5.60)| \leq \mathcal{K}(\varphi_t, A_t) \left(1 + \|A_t\|_{\frac{2p}{p-1}}\right) (\|q_1 \Psi_t\| + \|q_1 \Psi_t\|^2).$$

Therefore, if $A_t \in L^p(\mathbb{R}^2, \mathbb{C})$ holds for some $p \in]2, \infty]$ and for all $t \in \mathbb{R}$, we obtain

$$|\|\nabla_1 \Psi_t\|^2 - \|\nabla \varphi_t\|^2| \leq t \sup_{s \in [0, t]} \left(\mathcal{K}(\varphi_s, A_s) \left(\alpha(\Psi_s, \varphi_s) + \sqrt{\alpha(\Psi_s, \varphi_s)} + N^{-\delta} + N^{-1} \right) \right).$$

Since

$$\|\nabla_1 q_1 \Psi_t\|^2 \leq |\|\nabla_1 \Psi_t\|^2 - \|\nabla \varphi_t\|^2| + \|\nabla \varphi_t\|^2 \langle\Psi_t, q_1 \Psi_t\rangle + 2\|\nabla \varphi_t\| \|q_1 \Psi_t\| \|\Psi_t\|$$

holds, we obtain with part (a) of Theorem 5.2.2, part (b) of Theorem 5.2.2.

□

5.5 Appendix to Chapter 5

5.5.1 Energy variance of a product state

Lemma 5.5.1 *Let $\Psi = \varphi^{\otimes N}$ and assume that $\|\varphi\|_\infty + \|\Delta \varphi\|_\infty + \|\Delta \varphi\| + \|\nabla \varphi\| + \langle\varphi, A_s \varphi\rangle + \langle\varphi, A_s^2 \varphi\rangle \leq C$. Then,*

$$\text{Var}_{H_{W_\beta, s}}(\Psi) \leq C(N^{-1} + N^{-1+\beta} + N^{-2+2\beta}). \quad (5.61)$$

Proof: The proof is a direct calculation using the product structure of $\Psi = \varphi^{\otimes N}$. We first calculate, denoting $T = \sum_{k=1}^N (-\Delta_k)$, $\mathcal{W} = \sum_{i < j} W_\beta(x_i - x_j)$ and $\mathcal{A} = \sum_{k=1}^N A_s(x_k)$,

$$\begin{aligned} \frac{1}{N^2} \langle\Psi, H_{W_\beta, s} \Psi\rangle^2 &= \frac{1}{N^2} \langle\Psi, (T + \mathcal{W} + \mathcal{A}) \Psi\rangle^2 \\ &= \frac{1}{N^2} (N \langle\varphi, -\Delta \varphi\rangle + \frac{N(N-1)}{2} \langle\varphi, W_\beta * |\varphi|^2 \varphi\rangle + N \langle\varphi, A_s \varphi\rangle)^2 \\ &= \langle\varphi, -\Delta \varphi\rangle^2 + \frac{(N-1)^2}{4} \langle\varphi, W_\beta * |\varphi|^2 \varphi\rangle^2 + \langle\varphi, A_s \varphi\rangle^2 \\ &\quad + (N-1) \langle\varphi, -\Delta \varphi\rangle \langle\varphi, W_\beta * |\varphi|^2 \varphi\rangle + 2 \langle\varphi, -\Delta \varphi\rangle \langle\varphi, A_s \varphi\rangle \\ &\quad + (N-1) \langle\varphi, A_s \varphi\rangle \langle\varphi, W_\beta * |\varphi|^2 \varphi\rangle. \end{aligned}$$

It then follows that

$$\begin{aligned} \text{Var}_{H_{W_\beta,s}}(\Psi) &= \langle\langle \Psi, \frac{H_{W_\beta,s}^2}{N^2} \Psi \rangle\rangle - \frac{1}{N^2} \langle\langle \Psi, H_{W_\beta,s} \Psi \rangle\rangle^2 \\ &= \frac{1}{N^2} \langle\langle \Psi, T^2 \Psi \rangle\rangle - \langle \varphi, -\Delta \varphi \rangle^2 \end{aligned} \quad (5.62)$$

$$+ \frac{1}{N^2} 2\text{Re}(\langle\langle T\Psi, \mathcal{W}\Psi \rangle\rangle) - (N-1) \langle \varphi, -\Delta \varphi \rangle \langle \varphi, W_\beta * |\varphi|^2 \varphi \rangle \quad (5.63)$$

$$+ \frac{1}{N^2} \langle\langle \Psi, \mathcal{W}^2 \Psi \rangle\rangle - \frac{(N-1)^2}{4} \langle \varphi, W_\beta * |\varphi|^2 \varphi \rangle^2 \quad (5.64)$$

$$+ \frac{1}{N^2} \langle\langle \Psi, \mathcal{A}^2 \Psi \rangle\rangle - \langle \varphi, A_s \varphi \rangle^2 \quad (5.65)$$

$$+ \frac{1}{N^2} 2\text{Re}(\langle\langle \mathcal{A}\Psi, T\Psi \rangle\rangle) - 2 \langle \varphi, -\Delta \varphi \rangle \langle \varphi, A_s \varphi \rangle \quad (5.66)$$

$$+ \frac{1}{N^2} 2\text{Re}(\langle\langle \mathcal{A}\Psi, \mathcal{W}\Psi \rangle\rangle) - (N-1) \langle \varphi, W_\beta * |\varphi|^2 \varphi \rangle \langle \varphi, A_s \varphi \rangle. \quad (5.67)$$

We estimate each line separately.

$$\begin{aligned} |(5.62)| &= \left| \frac{1}{N} \langle\langle \Psi, (-\Delta_1)^2 \Psi \rangle\rangle + \frac{N-1}{N} \langle\langle \Psi, (-\Delta_1)(-\Delta_2) \Psi \rangle\rangle - \langle \varphi, -\Delta \varphi \rangle^2 \right| \\ &\leq \frac{\| -\Delta \varphi \|^2 + \|\nabla \varphi \|^4}{N}. \end{aligned}$$

Note that

$$\begin{aligned} \frac{1}{N^2} 2\text{Re}(\langle\langle T\Psi, \mathcal{W}\Psi \rangle\rangle) &= \frac{1}{N^2} \sum_{k=1}^N \sum_{i \neq j=1}^N \text{Re}(\langle\langle (-\Delta_k) \Psi, W_\beta(x_i - x_j) \Psi \rangle\rangle) \\ &= \frac{2(N-1)}{N} \text{Re}(\langle\langle (-\Delta_1) \Psi, W_\beta(x_1 - x_2) \Psi \rangle\rangle) \\ &\quad + \frac{(N-1)(N-2)}{N} \text{Re}(\langle\langle (-\Delta_1) \Psi, W_\beta(x_2 - x_3) \Psi \rangle\rangle) \\ &\leq \frac{2(N-1)}{N} \|\Delta \varphi\|_\infty \|W_\beta(x_1 - x_2)\|_1 \|\varphi\|_\infty \\ &\quad + \frac{(N-1)(N-2)}{N} \|\nabla \varphi\|^2 \langle \varphi, W_\beta * |\varphi|^2 \varphi \rangle \\ &\leq CN^{-1} \|\Delta \varphi\|_\infty \|\varphi\|_\infty + \frac{(N-1)(N-2)}{N} \langle \varphi, -\Delta \varphi \rangle \langle \varphi, W_\beta * |\varphi|^2 \varphi \rangle, \end{aligned}$$

which immediately implies

$$|(5.63)| \leq C \frac{\|\nabla \varphi\|_\infty \|\varphi\|_\infty + \|\nabla \varphi\|^2 \|\varphi\|_\infty^4}{N}.$$

Next, we calculate

$$\begin{aligned}
\frac{1}{N^2} \langle\langle \Psi, \mathcal{W}^2 \Psi \rangle\rangle &= \frac{1}{4N^2} \sum_{i \neq j=1}^N \sum_{k \neq l=1}^N \langle\langle \Psi, W_\beta(x_i - x_j) W_\beta(x_k - x_l) \Psi \rangle\rangle \\
&= \frac{N-1}{2N} \langle\langle \Psi, W_\beta(x_1 - x_2)^2 \Psi \rangle\rangle \\
&\quad + \frac{(N-1)(N-2)}{N} \langle\langle \Psi, W_\beta(x_1 - x_2) W_\beta(x_2 - x_3) \Psi \rangle\rangle \\
&\quad + \frac{(N-1)(N-2)(N-3)}{4N} \langle\langle \Psi, W_\beta(x_1 - x_2) W_\beta(x_3 - x_4) \Psi \rangle\rangle.
\end{aligned}$$

The first term is bounded by

$$\frac{N-1}{2N} \langle\langle \Psi, W_\beta(x_1 - x_2)^2 \Psi \rangle\rangle \leq \|\varphi\|_\infty^2 \|W_\beta\|^2 \leq CN^{-2+2\beta} \|\varphi\|_\infty^2.$$

The second term can be bounded using

$$\begin{aligned}
f(x_2) &= N^{-1+2\beta} \left| \int_{\mathbb{R}^2} dx_1 |\varphi(x_1)|^2 W(N^\beta(x_1 - x_2)) \right| \\
&\leq N^{-1} \int_{\mathbb{R}^2} dx_1 |\varphi(N^{-\beta}x_1)|^2 |W(x_1 - N^\beta x_2)| \leq N^{-1} \|W\|_1 \|\varphi\|_\infty^2
\end{aligned}$$

by

$$\begin{aligned}
&\frac{(N-1)(N-2)}{N} \langle\langle \Psi, W_\beta(x_1 - x_2) W_\beta(x_2 - x_3) \Psi \rangle\rangle \\
&= \frac{(N-1)(N-2)}{N} \int_{\mathbb{R}^2} dx_2 |\varphi(x_2)|^2 f(x_2)^2 \leq \frac{1}{N} \|W\|_1^2 \|\varphi\|_\infty^4.
\end{aligned}$$

It therefore follows that

$$|(5.64)| \leq CN^{-2+2\beta} \|\varphi\|_\infty^2 + CN^{-1} (\|\varphi\|_\infty^2 + \|\varphi\|_\infty^4).$$

(5.65) is estimated by

$$\begin{aligned}
|(5.65)| &= \left| \frac{1}{N} \langle\langle \Psi, A_s(x_1)^2 \Psi \rangle\rangle + \frac{N-1}{N} \langle\langle \Psi, A_s(x_1) A_s(x_2) \Psi \rangle\rangle - \langle\varphi, A_s \varphi\rangle^2 \right| \\
&\leq \frac{\langle\varphi, A_s^2 \varphi\rangle + \langle\varphi, A_s \varphi\rangle^2}{N}.
\end{aligned}$$

Furthermore,

$$\begin{aligned}
|(5.66)| &\leq \left| \frac{2}{N} |\langle\langle \Psi, A_s(x_1) (-\Delta_1) \Psi \rangle\rangle| + 2 \frac{N-1}{N} \langle\langle \Psi, A_s(x_1) (-\Delta_2) \Psi \rangle\rangle - 2 \langle\varphi, -\Delta \varphi\rangle \langle\varphi, A_s \varphi\rangle \right| \\
&\leq C \frac{\|-\Delta \varphi\| \|A_s \varphi\| + \|\nabla \varphi\|^2 \langle\varphi, A_s \varphi\rangle}{N}.
\end{aligned}$$

Finally,

$$\begin{aligned}
 |(5.67)| &\leq C (|\langle A_s(x_1)\Psi, W_\beta(x_1 - x_2)\Psi \rangle| + |\langle \Psi, A_s(x_1)W_\beta(x_2 - x_3)\Psi \rangle|) \\
 &\leq C(\|A_s\varphi\| \|W_\beta\| \|\varphi\|_\infty + \langle \varphi, A_s\varphi \rangle \|W_\beta\|_1 \|\varphi\|_\infty^2) \\
 &\leq C(N^{-1+\beta} \|A_s\varphi\| \|\varphi\|_\infty + N^{-1} \langle \varphi, A_s\varphi \rangle \|\varphi\|_\infty^2).
 \end{aligned}$$

□

5.5.2 Persistence of regularity of φ_t

We study the nonlinear Schrödinger equation in two spatial dimensions (5.3) with a harmonic potential

$$i\partial_t\varphi_t = (-\Delta + a|\varphi_t|^2 + |x|^2)\varphi_t \quad (5.68)$$

under the conditions $a > -a^*$ and $\|\varphi_0\| = 1$. The solution theory of (5.3) is well studied in absence of external fields. There, the global existence and persistence of regularity of $\varphi_t \in H^k(\mathbb{R}^2, \mathbb{C})$ was established, assuming φ_0 regular enough [12]. The condition $a > -a^*$ is known to be optimal, that is, for $a < -a^*$, there exist blow-up solutions. It is interesting to note that global existence of solutions in $L^\infty(\mathbb{R}^2, \mathbb{C})$ directly implies persistence of higher regularity of solutions in $H^k(\mathbb{R}^2, \mathbb{C})$, see [12] and below.

Lemma 5.5.2 *Let $\varphi_0 \in H^1(\mathbb{R}^2, \mathbb{C})$, $\|\varphi_0\| = 1$ such that $\|\nabla\varphi_0\|^2 + \||x|\varphi_0\|^2 + \frac{a}{2}\langle\varphi_0, |\varphi_0|^2\varphi_0\rangle \leq C$. Let $a > -a^*$.*

(a) *The nonlinear Schrödinger equation*

$$i\partial_t\varphi_t = (-\Delta + a|\varphi_t|^2 + |x|^2)\varphi_t$$

admits a solution $\varphi_t \in H^1(\mathbb{R}^2, \mathbb{C})$ globally in time.

(b) *Define the norm $\|u\|_{\Sigma,m} = \sqrt{\sum_{k=0}^m (\|\nabla^k u\|^2 + \||x|^k u\|^2)}$. Then*

$$\|\varphi_t\|_{\Sigma,4} \leq \|\varphi_0\|_{\Sigma,4} e^{C \int_0^t ds \|\varphi_s\|_\infty^2}.$$

(c) *Assume $\|\varphi_0\|_{\Sigma,4} < \infty$. Then, there exist a time-dependent constant C_t , also depending on $\|\varphi_0\|_{\Sigma,4}$, such that $\|\varphi_t\|_{\Sigma,4} \leq C_t$.*

Remark 5.5.3 *Part (c) directly implies that $\varphi_t \in H^4(\mathbb{R}^2, \mathbb{C})$. Our proof relies on the works of [10, 11, 12, 29, 69, 71], see also the references therein. It also might be possible to show a polynomial growth in t of the constant C_t , using the refined estimates presented in [10, 11].*

Proof:

(a) The global existence in $H^1(\mathbb{R}^2, \mathbb{C})$ is well known, see Remark 3.6.4 in [12]. We sketch the proof for completeness. Let U_t denote the generator of the time evolution of the linear Schrödinger equation $i\partial_t u_t = (-\Delta + |x|^2)u_t$. For any $\varphi_0 \in L^2(\mathbb{R}^2, \mathbb{C})$, we consider the Duhamel formula

$$\varphi_t = U_t \varphi_0 - ia \int_0^t ds U_{t-s} |\varphi_s|^2 \varphi_s. \quad (5.69)$$

Note that it is known that there exists a nonempty open interval I , $0 \in I$ such that (5.69) has a unique solution φ_t , provided the initial datum φ_0 fulfills $\|\varphi_0\|_{\Sigma,1} \leq C$ (see Proposition 1.5. in [11]). Furthermore, for any $t \in I$, $\|\varphi_t\| = \|\varphi_0\| = 1$. We may assume that I is the maximal interval on which a solution of (5.69) exists. Assume now that φ_t blows up in finite time, i.e. I is bounded. It is then known that $\int_0^{\sup I} dt \|\varphi_t\|_4^4 = \infty$ [29].

Assume $t \in I$ and consider the NLS energy

$$\mathcal{E}_{\text{NLS}}(\varphi_t) = \|\nabla \varphi_t\|^2 + \frac{a}{2} \langle \varphi_t, |\varphi_t|^2 \varphi_t \rangle + \||x|\varphi_t\|^2.$$

Under the conditions $a > -a^*$, $\|\varphi_0\| = 1$, the two dimensional Gagliardo-Nirenberg inequality $\frac{a^*}{2} \|u\|_4^4 \leq \|\nabla u\|^2 \|u\|^2$, $u \in H^1(\mathbb{R}^2, \mathbb{C})$ implies that $\mathcal{E}_{\text{NLS}}(\varphi_t) > 0$. Furthermore $\frac{d}{dt} \mathcal{E}_{\text{NLS}}(\varphi_t) = 0$, see Proposition 1.6. in [11]. This directly implies that there exists an $\epsilon > 0$ such that

$$\epsilon \|\nabla \varphi_t\|^2 \leq C.$$

The two dimensional Gagliardo-Nirenberg inequality implies, together with $\|\varphi_t\| = \|\varphi_0\|$, $\forall t \in I$,

$$\int_0^{\sup I} dt \|\varphi_t\|_4^4 \leq C \int_0^{\sup I} dt \|\nabla \varphi_t\|^2 \leq C \sup I < \infty.$$

Therefore, the solution φ_t of (5.69) exists globally in time and fulfills $\varphi_t \in H^1(\mathbb{R}^2, \mathbb{C})$, $\||x|\varphi_t\| < \infty$.

(b) Let $A(x) = |x|^2$ and define, for any $u \in L^2(\mathbb{R}^2, \mathbb{C})$, the norm

$$\|u\|_{k,A} = \sqrt{\sum_{m=0}^k \|(-\Delta + A)^m u\|^2}.$$

Note that $\|\cdot\|_{k,A}$ is invariant under U_t , that is $\|U_t u\|_{k,A} = \|u\|_{k,A}$. We will first show that $\|u\|_{2,A}$ and $\|u\|_{\Sigma,4}$ are equivalent norms. Let $u \in H^4(\mathbb{R}^2, \mathbb{C})$. Note that

$$\begin{aligned} \|u\|_{2,A}^2 &= \|u\|^2 + \|(-\Delta + A)u\|^2 + \|(-\Delta + A)^2 u\|^2 \\ &\leq \|u\|^2 + 2\|-\Delta u\|^2 + 2\|Au\|^2 \\ &\quad + \left\| \left((-\Delta)^2 + A^2 + (-\Delta A) + 2A(-\Delta) - 2(\nabla A) \cdot \nabla \right) u \right\|^2 \\ &\leq C \left(\|u\|^2 + \|-\Delta u\|^2 + \|Au\|^2 + \|(-\Delta)^2 u\|^2 + \|A^2 u\|^2 \right. \\ &\quad \left. + \|A(-\Delta)u\|^2 + \|(\nabla A) \cdot \nabla u\|^2 \right). \end{aligned}$$

Since $\nabla A^2 = 4|x|^2 x$, $\Delta A^2 = 12A$, we obtain,

$$\begin{aligned}\|A(-\Delta)u\|^2 &= \langle u, (-\Delta)A^2(-\Delta)u \rangle \\ &= \langle u, (-\Delta A^2)(-\Delta)u \rangle + 2\langle u, (-\nabla A^2) \cdot \nabla(-\Delta)u \rangle + \langle u, A^2(-\Delta)^2u \rangle \\ &\leq C(\|Au\| \| -\Delta u \| + \||x|^3 u\| \|\nabla \Delta u\| + \|A^2 u\| \|(-\Delta)^2 u\|) \\ &\leq C(\|Au\|^2 + \| -\Delta u \|^2 + \|(-\Delta)^2 u \|^2 + \|A^2 u\|^2).\end{aligned}$$

For the last inequality, we used $\||x|^3 u\|^2 = \langle |x|^2 u, |x|^4 u \rangle \leq \|Au\|^2 + \|A^2 u\|^2$, as well as $\|\nabla \Delta u\| \leq \| -\Delta u \|^2 + \|(-\Delta)^2 u \|^2$. We use polar coordinates (r, φ) . Then, $(\nabla A) \cdot \nabla = 2r\partial_r$. Hence,

$$\begin{aligned}\|(\nabla A) \cdot \nabla u\|^2 &= -4\langle u, \partial_r(r^2\partial_r u) \rangle = -4\langle u, (2r\partial_r + r^2\partial_r^2) u \rangle \\ &= -4\langle u, r^2(r^{-1}\partial_r + \partial_r^2) u \rangle - 4\langle u, r\partial_r u \rangle \\ &\leq 4\langle r^2 u, -\left(r^{-1}\partial_r + \partial_r^2 + \frac{1}{r^2}\partial_\varphi^2\right) u \rangle - 4\left\langle |x| \frac{x}{|x|} u, \nabla u \right\rangle \\ &\leq C(\|Au\|^2 + \| -\Delta u \|^2 + \||x| u\|^2 + \|\nabla u\|^2).\end{aligned}$$

Therefore, $\|u\|_{2,A} \leq C\|u\|_{\Sigma,4}$ holds. To show the converse, first note that $\|u\|_{\Sigma,4}^2 \leq C(\|u\|^2 + \|Au\|^2 + \| -\Delta u \|^2 + \|A^2 u\|^2 + \|\Delta^2 u\|^2)$. Since $-\Delta \leq -\Delta + |x|^2$ and $|x|^2 \leq -\Delta + |x|^2$ holds as an operator inequality, we directly obtain $\|u\|_{\Sigma,4} \leq C\|u\|_{2,A}$.

By $\|uv\|_{H^k} \leq \|u\|_\infty \|v\|_{H^k} + \|u\|_{H^k} \|v\|_\infty$, $\|\cdot\|_{2,A}$ fulfills the generalized Leibniz rule

$$\begin{aligned}\|uv\|_{2,A} &\leq C\|uv\|_{\Sigma,4} \leq C(\|u\|_\infty \|v\|_{\Sigma,4} + \|u\|_{\Sigma,4} \|v\|_\infty) \\ &\leq C(\|u\|_{2,A} \|v\|_\infty + \|u\|_\infty \|v\|_{2,A}).\end{aligned}$$

From (5.69), we obtain

$$\begin{aligned}\|\varphi_t\|_{2,A} &\leq \|U_t \varphi_0\|_{2,A} + |a| \int_0^t ds \|U_{t-s} |\varphi_s|^2 \varphi_s\|_{2,A} \\ &= \|\varphi_0\|_{2,A} + |a| \int_0^t ds \|\varphi_s\|_{2,A}^2 \\ &\leq \|\varphi_0\|_{2,A} + C \int_0^t ds \|\varphi_s\|_\infty^2 \|\varphi_s\|_{2,A}.\end{aligned}$$

By a Grönwall inequality, we obtain (b).

(c) We show that $\varphi_t \in H^2(\mathbb{R}^2, \mathbb{C})$ globally in time. Recall the existence of global in time solutions of

$$i\partial_t u_t = (-\Delta + a|u_t|^2)u_t. \quad (5.70)$$

in $H^2(\mathbb{R}^2, \mathbb{C})$, provided that $a > -a^*$ and $u_0 \in H^2(\mathbb{R}^2, \mathbb{C})$, $\|u_0\| = 1$ holds. Using the lens transform [10, 69], for $|t| < \pi/2$

$$\varphi_t(x) = \frac{1}{\cos(t)} u_{\tan(t)} \left(\frac{x}{\cos(t)} \right) e^{-i \frac{|x|^2}{2} \tan(t)},$$

φ_t then solves $i\partial_t \varphi_t = (-\Delta + a|\varphi_t|^2 + |x|^2)\varphi_t$ with initial datum $\varphi_0 = u_0$. We therefore see that the existence of a global-in-time solution of (5.70) in $H^2(\mathbb{R}^2, \mathbb{C})$ implies existence of a solution φ_t in $H^2(\mathbb{R}^2, \mathbb{C})$ locally in $t \in]-\pi/2, \pi/2[$. By translation invariance of time, the solution φ_t then exists globally in $H^2(\mathbb{R}^2, \mathbb{C})$. By the embedding $L^\infty(\mathbb{R}^2, \mathbb{C}) \subset H^2(\mathbb{R}^2, \mathbb{C})$, we obtain, together with (b), (c).

□

5.5.3 Self-Adjointness

Lemma 5.5.4 *Let*

$$H_{W_\beta, t} = \sum_{k=1}^N (-\Delta_k) + \sum_{i < j=1}^N W_\beta(x_i - x_j) + \sum_{k=1}^N A_t(x_k)$$

and assume (A1) and (A2). Then, for all $t \in \mathbb{R}$,

- (a) $H_{W_\beta, t}$ is selfadjoint with domain $\mathcal{D}(H_{W_\beta, t}) = \mathcal{D}\left(\sum_{k=1}^N (-\Delta_k + A_0(x_k))\right)$.
- (b) $(H_{W_\beta, t})^2$ is selfadjoint with domain $\mathcal{D}((H_{W_\beta, t})^2) = \mathcal{D}((H_{W_\beta, 0})^2)$. If, in addition, $W \in C^2(\mathbb{R}^2, \mathbb{R})$, then $\mathcal{D}((H_{W_\beta, t})^2) = \mathcal{D}\left(\left(\sum_{k=1}^N (-\Delta_k + A_0(x_k))\right)^2\right)$ holds.

Proof:

- (a) First note that $\mathcal{D}(H_{W_\beta, 0}) = \mathcal{D}\left(\sum_{k=1}^N (-\Delta_k + A_0(x_k))\right)$, since $W_\beta \in L_c^\infty(\mathbb{R}^2, \mathbb{R})$. We write

$$H_{W_\beta, t} = H_{W_\beta, 0} + \sum_{k=1}^N \int_0^t ds \dot{A}_s(x_k).$$

Abbreviate $\mathcal{A}_t = \sum_{k=1}^N \int_0^t ds \dot{A}_s(x_k)$. Since $\|\mathcal{A}_t \Psi\| \leq N \int_0^t ds \|\dot{A}_s\|_\infty \|\Psi\|$ holds for all $\Psi \in L^2(\mathbb{R}^2, \mathbb{C})$, \mathcal{A}_t is infinitesimal $H_{W_\beta, 0}$ bounded, which implies by Kato-Rellich that $\mathcal{D}(H_{W_\beta, 0}) = \mathcal{D}(H_{W_\beta, t})$.

- (b) Note that $(H_{W_\beta, 0})^2$ is self-adjoint on $\mathcal{D}((H_{W_\beta, 0})^2)$. Consider

$$(H_{W_\beta, t})^2 = (H_{W_\beta, 0})^2 + H_{W_\beta, 0} \mathcal{A}_t + \mathcal{A}_t H_{W_\beta, 0} + \mathcal{A}_t^2.$$

Under Assumption (A2), $H_{W_\beta,0}\mathcal{A}_t + \mathcal{A}_t H_{W_\beta,0} + \mathcal{A}_t^2$ is a symmetric operator on $\mathcal{D}((H_{W_\beta,0})^2)$. We estimate, for $\Psi \in \mathcal{D}((H_{W_\beta,0})^2)$, $\Psi \neq 0$,

$$\begin{aligned} & \| (H_{W_\beta,0}\mathcal{A}_t + \mathcal{A}_t H_{W_\beta,0} + (\mathcal{A}_t)^2) \Psi \| \\ & \leq 2N \int_0^t ds \|\dot{A}_s\|_\infty \|H_{W_\beta,0}\Psi\| + N^2 \left(\int_0^t ds \|\dot{A}_s\|_\infty \right)^2 \|\Psi\| \\ & + N \int_0^t ds \|\Delta \dot{A}_s\|_\infty \|\Psi\| + 2 \left\| \sum_{k=1}^N \int_0^t ds \nabla_k \dot{A}_s(x_k) \nabla_k \Psi \right\| \end{aligned}$$

Note that

$$\begin{aligned} 2N \int_0^t ds \|\dot{A}_s\|_\infty \|H_{W_\beta,0}\Psi\| &= 2N \int_0^t ds \|\dot{A}_s\|_\infty \sqrt{\langle\langle \Psi, (H_{W_\beta,0})^2 \Psi \rangle\rangle} \\ &\leq \sqrt{2N^2 \left(\int_0^t ds \|\dot{A}_s\|_\infty \right)^2 \|\Psi\|^2 + \frac{1}{2} \left\| (H_{W_\beta,0})^2 \Psi \right\|^2} \\ &\leq \sqrt{2N} \int_0^t ds \|\dot{A}_s\|_\infty \|\Psi\| + \frac{1}{\sqrt{2}} \left\| (H_{W_\beta,0})^2 \Psi \right\|. \end{aligned}$$

Furthermore, for $\epsilon > 0$

$$\begin{aligned} 2 \left\| \sum_{k=1}^N \int_0^t ds \nabla_k \dot{A}_s(x_k) \nabla_k \Psi \right\| &\leq 2 \sum_{k=1}^N \int_0^t ds \|\nabla \dot{A}_s\|_\infty \|\nabla_k \Psi\| \\ &\leq \frac{2N}{\epsilon} \left(\int_0^t ds \|\nabla \dot{A}_s\|_\infty \right)^2 \|\Psi\| + \frac{\epsilon}{2\|\Psi\|} \sum_{k=1}^N \|\nabla_k \Psi\|^2 \\ &\leq \frac{2N}{\epsilon} \left(\int_0^t ds \|\nabla \dot{A}_s\|_\infty \right)^2 \|\Psi\| + \frac{1}{2\|\Psi\|} \langle \Psi, H_{W_\beta,0}\Psi \rangle + CN\|\Psi\|. \end{aligned}$$

Since

$$\|\Psi\|^{-1} \langle\langle \Psi, H_{W_\beta,0}\Psi \rangle\rangle \leq \frac{1}{2} \|\Psi\| + \frac{1}{2\|\Psi\|} \|H_{W_\beta,0}\Psi\|^2 \leq \|\Psi\| + \frac{1}{2} \|(H_{W_\beta,0})^2 \Psi\|,$$

we obtain

$$\begin{aligned} & \| (H_{W_\beta,0}\mathcal{A}_t + \mathcal{A}_t H_{W_\beta,0} + (\mathcal{A}_t)^2) \Psi \| \leq \left(\frac{1}{\sqrt{2}} + \frac{1}{4} \right) \|(H_{W_\beta,0})^2 \Psi\| \\ & + \left(\sqrt{2N} \int_0^t ds \|\nabla \dot{A}_s\|_\infty + \frac{2N}{\epsilon} \left(\int_0^t ds \|\nabla \dot{A}_s\|_\infty \right)^2 + CN \right) \|\Psi\| \\ & + N \int_0^t ds \|\Delta \dot{A}_s\|_\infty \|\Psi\|. \end{aligned}$$

Thus, $H_{W_\beta,0}\mathcal{A}_t + \mathcal{A}_t H_{W_\beta,0} + (\mathcal{A}_t)^2$ is relatively $(H_{W_\beta,0})^2$ bounded with bound $\frac{1}{\sqrt{2}} + \frac{1}{4} < 1$. By Kato-Rellich, $(H_{W_\beta,t})^2$ is self-adjoint with domain $\mathcal{D}((H_{W_\beta,t})^2) = \mathcal{D}((H_{W_\beta,0})^2)$, for all $t \in \mathbb{R}$. By a similar estimate, we also obtain

$$\mathcal{D}((H_{W_\beta,0})^2) = \mathcal{D}\left(\left(\sum_{k=1}^N (-\Delta_k + A_0(x_k))^2\right)\right),$$

if $W \in C^2(\mathbb{R}^2, \mathbb{C})$.

□

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Eidesstattliche Versicherung

(Siehe Promotionsordnung vom 12.07.11, §8, Abs. 2 Pkt. 5)

Hiermit erkläre ich an Eidesstatt, dass die Dissertation von mir selbstständig, ohne unerlaubte Beihilfe angefertigt ist. Kapitel 4 und 5 enthalten Resultate, die aus einer Zusammenarbeit mit Prof. Dr. Peter Pickl stammen. Kapitel 3 entält Resultate, die aus einer Zusammenarbeit mit Prof. Dr. Peter Pickl und Dr. Nikolai Leopold stammen. Die von mir zu den Veröffentlichungen geleisteten Beiträge werden am Anfang der entsprechenden Kapitel aufgeführt.

München, den 03. April 2018

Maximilian Jeblick

