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Mean Field Limits in Bosonic Systems

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Abstract

Via mean field theory, we analyze the time evolution of a system consisting of one, respectively two distinguishable types of bosons being initially in an almost product state. Assuming that interaction takes place between all pairs of particles, we prove that the property of an almost product state is conserved for all finite times. Moreover, it is feasible to stretch this statement to all times under additional assessments. In the outlook, we give reasons, why this approach does not work for one species of bosons in two different states.

This thesis is a generalization of the method of counting bad particles which was introduced in [3].

Part I

Introduction

We study the time evolution of an N -particle bosonic system in the mean field limit. Initially, we create an N -particle state in which most of the bosons are supposed to be independently from each other in the same one-particle state $\varphi \in L^2(\mathbb{R}^3) \cap L^{2s}(\mathbb{R}^3)$, where $s \in [1, \infty)$. Therefore, we take for granted that the normalized N -particle state $\Psi_N \in L^2(\mathbb{R}^{3N})$ has the structure of an (almost) product state. Besides, the particles in our system move in a time dependent external potential and interact pairwise between each other. Consequently, the corresponding Hamiltonian of the bosonic system looks like

$$H_N = \sum_{j=1}^N (-\Delta_j) + \sum_{j=1}^N A^t(x_j) + \sum_{1 \leq j < k \leq N} V_N(x_j - x_k). \quad (1)$$

We prove under these assumptions, that the N -particle state Ψ_N keeps its (almost) product structure in the mean field limit for all finite times, although there is pair interaction and therefore correlation between the bosons.

In order to verify this assertion, we show Ψ_N being an (almost) product state is in the mean field limit equivalent to the convergence to 0 of the number of particles which are not in the state φ in which we want them to be. The goal is to prove that the amount of these so called *bad particles* converges for all finite times in the mean field limit to 0. Moreover, the proof includes at the same time the verification of the Hartree equation which reflects the dynamics of one single particle.

To be continued, we apply this method of counting bad particles to another system which consists of two distinguishable types of bosons where pair interaction takes place between all particles. We show that its wave function also conserves the (almost) product structure under these assumptions.

Finally, we give some reasons, why the application of this method to a system consisting of one type of particles in two different states is really hard work.

Part II

Time Evolution of Identical Bosons

1 Definitions and Properties

In this section, we prove for all finite times the equivalence of Ψ_N^t is an almost product state, the reduced density matrix converges to the pure state φ^t in operator norm and the ratio of bad particles converges in the mean field limit to 0, i.e.

$$\Psi_N^t \text{ almost product state} \Leftrightarrow \begin{array}{c} \mu^{\Psi_N^t} \xrightarrow{N \rightarrow \infty} |\varphi^t\rangle \langle \varphi^t| \\ \text{in operator norm} \end{array} \Leftrightarrow \omega^{\varphi^t} \xrightarrow{N \rightarrow \infty} 0. \quad (2)$$

(i) (ii) (iii)

Later on, we show that (ii) is a consequence of (i), (ii) and (iii) are equivalent and (i) follows from (iii).

We know that Ψ_N has to be symmetric under particle exchange since we look at a bosonic many-particle system. Therefore

$$\Psi_N^t(x_1, \dots, x_i, \dots, x_j, \dots, x_N) = \Psi_N^t(x_1, \dots, x_j, \dots, x_i, \dots, x_N) \quad (3)$$

holds for every $i, j \in \{1, \dots, N\}$.

1.1 The reduced one-particle density matrix μ^{Ψ_N}

Up to now, no theoretical or mathematical physicist is talking about counting bad particles or treating an almost product state when considering the time evolution of systems in the mean field limit, which was introduced in [3]. The common physical world uses the reduced one-particle density matrix.

Definition:

Let $\Psi_N \in L^2(\mathbb{R}^{3N})$ represent a normalized N -particle state. The reduced one-particle density matrix is defined as:

$$\mu^{\Psi_N}(x, y) := \int \Psi_N(x, x_2, \dots, x_N) \Psi_N^*(y, x_2, \dots, x_N) dx_2 \dots dx_N \quad (4)$$

In the following, we neglect for convenience the dimension of the integral, i.e. dx_k means d^3x_k .

However, the reduced one-particle density matrix does not describe our system in detail, i.e. we cannot determine the structure or any other properties of Ψ_N . The reason for the loss of information is the integration over $N-1$ variables. Consequently, one should not refer to the reduced one-particle density matrix in order to explain the time evolution of the bosonic system, since we want to determine the structure of the N -particle wave function.

Nevertheless, since physicists like talking about μ^{Ψ_N} , we always build bridges from the method of counting bad particles as well as the N -particle state to the reduced one-particle density matrix.

1.2 The (almost) product state and bad particles

In order to repeat the question from the introduction, we prove that an (almost) product state conserves its structure although there is pair interaction between the bosons. Because of this, we firstly have to declare the properties of an almost product state.

If the N-particle state can be written as product of all one-particle states φ

$$\Psi_N(x_1, \dots, x_N) = \prod_{j=1}^N \varphi(x_j) \quad (5)$$

then for sure the equality

$$\mu^{\Psi_N}(x, y) = \varphi(x)\varphi^*(y) \quad (6)$$

holds. We call (5) a product state. Physically, a system in such a state consists of N subsystems which are totally independent of each other, so the particles do not influence each other. For that reason, there exists no interaction between these bosons and consequently the particles are not correlated, i.e. every particle itself lives for its-own.

Moreover, in experimental physics it is not possible to realize N identical one-particle states called φ even if we treat a Bose-Einstein-Condensate. Note, the ratio of bosons of an ideal Bose-Gas which are in the ground state of an N-particle system is based on the absolute temperature in the following way

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_B} \right)^{\frac{3}{2}} \quad (7)$$

where T_B is the bose temperature, i.e. the Bose-Einstein-Condensate appears for $T < T_B$ (cf. [1] headword: Bose-Einstein-Kondensation). Up to now, in experimental physics, we cannot reach the absolute temperature zero point and consequently there always exist particles which are not in the ground state. Nevertheless, we assume that this number n is much smaller than the number of all bosons. Furthermore, we are not considering ideal gases, consequently there are always particles which are not in the state φ in which we want them to be. Therefore, these bosons are called *bad particles* or *bad bosons*. We sum them up to be in the symmetric, orthogonal and normalized state $\chi \in L^2(\mathbb{R}^{3n})$. Here the orthogonality is meant to be

$$\int \chi^*(\dots, x_k, \dots) \varphi(x_k) dx_k = 0. \quad (8)$$

An N-particle almost product state with $n \ll N$ bad particles looks like

$$\Psi_N = \frac{1}{\sqrt{\binom{N}{n}}} \left(\chi(x_1, \dots, x_n) \cdot \prod_{j=n+1}^N \varphi(x_j) \right)_{sym.} \quad (9)$$

which is normalized to one in $L^2(\mathbb{R}^{3N})$ norm. Here the index *sym.* assures that Ψ_N is symmetric and that is the reason, why the bosonic character is conserved. In order to emphasize its meaning, (9) consists of a sum of all possibilities to distribute n bad particles to N slots representing the N particles, which are at all $\binom{N}{n}$ summands. The binomial coefficient is defined as

$$\binom{N}{n} := \frac{N!}{(N-n)! \cdot n!} \quad (10)$$

1.3 From an (almost) product state Ψ_N to the convergence of μ^{Ψ_N}

Next, we prove by hand, that for an almost product state, the reduced one-particle density matrix converges in operator norm in the mean field limit $N \rightarrow \infty$, i.e.

$$\mu^{\Psi_N}(x, y) \xrightarrow{N \rightarrow \infty} \varphi(x)\varphi^*(y) \quad \text{in operator norm} \quad (11)$$

holds true. As a consequence, we compute

$$\begin{aligned} \mu^{\Psi_N}(x_1) &= \frac{1}{\binom{N}{n}} \int \left(\chi(x_1, \dots, x_n) \cdot \prod_{k=n+1}^N \varphi(x_k) \right)_{sym.} \\ &\quad \times \left(\chi^*(x_1, \dots, x_n) \cdot \prod_{k=n+1}^N \varphi^*(x_k) \right)_{sym.} dx_2 \dots dx_N \\ &= \frac{1}{\binom{N}{n}} \left\{ \binom{N-1}{n} \varphi(x_1)\varphi^*(x_1) \right. \\ &\quad \left. + \binom{N-1}{n-1} \int \chi(x_1, x_2, \dots, x_n) \chi^*(x_1, x_2, \dots, x_n) dx_2 \dots dx_n \right\} \\ &= \left(1 - \frac{n}{N}\right) \varphi(x_1)\varphi^*(x_1) + \frac{n}{N} \int \chi(x_1, x_2, \dots, x_n) \chi^*(x_1, x_2, \dots, x_n) dx_2 \dots dx_n \\ &\xrightarrow{N \rightarrow \infty} \varphi(x_1)\varphi^*(x_1) \quad \text{in operator norm} \end{aligned} \quad (12)$$

where we used that only the diagonal terms of the product contribute and the general fact that $\binom{N}{n} = \binom{N-1}{n} + \binom{N-1}{n-1}$ holds true. The first summand in (12) represents those diagonal terms in which x_1 is a good particle, whereas the second one stands for those diagonal terms in which x_1 is a bad particle.

Since the reduced one-particle density matrix above already converges in absolute value to the pure state φ , it also converges in operator norm. For clearness, we write it in detail, but for convenience we replace the integral by R .

$$\left\| \left(1 - \frac{n}{N}\right) |\varphi\rangle\langle\varphi| + \frac{n}{N} R - |\varphi\rangle\langle\varphi| \right\|_{op} = \frac{n}{N} \|R - |\varphi\rangle\langle\varphi|\|_{op} = \frac{n}{N} \quad (13)$$

The norm is equal to one because when the difference of operators acts on a normalized linear combination of φ and an eigenstate of R with eigenvalue one, we receive again a state which is normalized to one. Applying now the mean field limit $N \rightarrow \infty$ proves the circumstance given above. In fact, an almost product state consists of correlated particles, however, we can neglect the correlation in the mean field limit. Consequently, an almost product state has in the mean field limit the same properties as a product state.

1.4 The counting measure ω^φ

In the following, we introduce a mechanism which allows us to determine the number of bad particles given an N -particle state Ψ_N . Therefore, we sandwich the corresponding reduced one-particle matrix with φ , then we use Fubini to interchange the integrals. At the end we receive an expression which can by introducing a new projector be interpreted as an object counting bad particles.

$$\begin{aligned}
& \langle \varphi(x) | \mu^{\Psi_N}(x, y) | \varphi(y) \rangle \\
&= \int_x \varphi^*(x) \int_{x_2, \dots, x_N} \Psi_N(x, x_2, \dots, x_N) dx \int_y \Psi_N^*(y, x_2, \dots, x_N) dx_2 \dots dx_N \varphi(y) dy \\
&= \int_{x_2, \dots, x_N} \int_y \Psi_N^*(y, x_2, \dots, x_N) \varphi(y) dy \int_x \varphi^*(x) \Psi_N(x, x_2, \dots, x_N) dx \cdot dx_2 \dots dx_N \\
&= \langle \langle \Psi_N | \varphi \rangle \langle \varphi | \Psi_N \rangle \rangle
\end{aligned} \tag{14}$$

We assume φ and Ψ_N are nice functions and therefore we can use Fubini to interchange the integrals. In addition $\langle \langle \cdot | \cdot \rangle \rangle$ is the scalar product defined in $L^2(\mathbb{R}^{3N} \times \mathbb{R}^{3N}) \rightarrow \mathbb{C}$, whereas $\langle \cdot | \cdot \rangle$ is the scalar product on $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$. Let us define the projectors $p_i^\varphi, q_i^\varphi : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$ which act on the particle x_i

$$\begin{aligned}
p_i^\varphi &:= |\varphi(x_i)\rangle \langle \varphi(x_i)| = \varphi(x_i) \langle \varphi(x_i) | \cdot \rangle \\
q_i^\varphi &:= 1 - p_i^\varphi.
\end{aligned} \tag{15}$$

Notice that q_i^φ and p_i^φ are orthogonal, i.e. $q_i^\varphi p_i^\varphi = p_i^\varphi q_i^\varphi = 0$. As a consequence, (14) can be written as

$$\begin{aligned}
\langle \varphi | \mu^{\Psi_N} | \varphi \rangle &= \langle \varphi(x_1) | \Psi_N(x_1, x_2, \dots, x_N) \rangle \langle \langle \Psi_N(x_1, x_2, \dots, x_N) | \varphi(x_1) \rangle \rangle \\
&= \langle \langle \Psi_N(x_1, x_2, \dots, x_N) | \varphi(x_1) \rangle \langle \varphi(x_1) | \Psi_N(x_1, x_2, \dots, x_N) \rangle \rangle \\
&= \langle \langle \Psi_N | p_1^\varphi | \Psi_N \rangle \rangle \\
&= 1 - \langle \langle \Psi_N | q_1^\varphi | \Psi_N \rangle \rangle \\
&=: 1 - \omega^\varphi.
\end{aligned} \tag{16}$$

Due to the symmetry of Ψ_N concerning particle exchange, we can rewrite ω^φ by replacing q_1^φ by $\sum_{j=1}^N \frac{1}{N} q_j^\varphi$. Therefore the following equation holds true

$$\begin{aligned}
\omega^\varphi &= \langle \langle \Psi_N | q_1^\varphi | \Psi_N \rangle \rangle \\
&= \langle \langle \Psi_N | q_i^\varphi | \Psi_N \rangle \rangle \\
&= \left\langle \left\langle \Psi_N \left| \frac{1}{N} \cdot N q_i^\varphi \right| \Psi_N \right\rangle \right\rangle \\
&= \left\langle \left\langle \Psi_N \left| \frac{1}{N} \sum_{j=1}^N q_j^\varphi \right| \Psi_N \right\rangle \right\rangle \\
&= \frac{1}{N} \sum_{j=1}^N \langle \langle \Psi_N | q_j^\varphi | \Psi_N \rangle \rangle.
\end{aligned} \tag{17}$$

On this line, one can see that ω^φ is a counting measure, determining the ratio of particles which are not in the state φ , compared to the whole number of particles. Since we treat a bosonic system, it gives the ratio of bad particles compared to the number of all bosons and not the bad particles itself.

The counting measure ω^φ is a tool which determines the distance between an almost product state and a product state. Furthermore, one can think about a deviation in L^2 -sense, however, this is in our consideration too strong. We want to have a statement about how far we are away

from a product state. In order to illustrate this issue, we compute the difference in L^2 -norm of an N -particle product state and an N -particle state with n bad bosons.

$$\begin{aligned}
& \left\| \prod_{j=1}^N \varphi(x_j) - \frac{1}{\sqrt{\binom{N}{n}}} \left(\chi(x_1, \dots, x_n) \cdot \prod_{j=n+1}^N \varphi(x_j) \right) \right\|_{sym.}^2 \\
&= \int \left| \prod_{j=1}^N \varphi(x_j) - \frac{1}{\sqrt{\binom{N}{n}}} \left(\chi(x_1, \dots, x_n) \prod_{k=n+1}^N \varphi(x_k) \right) \right|_{sym.}^2 dx_1 \dots dx_N \\
&= \int \left\{ \prod_{j=1}^N |\varphi(x_j)|^2 - 2Re \left(\prod_{j=1}^N \varphi^*(x_j) \frac{1}{\sqrt{\binom{N}{n}}} \left(\chi(x_1, \dots, x_n) \prod_{k=n+1}^N \varphi(x_k) \right) \right) \right. \\
&\quad \left. + \left| \frac{1}{\sqrt{\binom{N}{n}}} \left(\chi(x_1, \dots, x_n) \prod_{k=n+1}^N \varphi(x_k) \right) \right|_{sym.}^2 \right\} dx_1 \dots dx_N \\
&= 2 = \text{constant}. \tag{18}
\end{aligned}$$

Here, the constant result just reflects that Ψ_N is not a product state since there is no dependency on n or N . In contrast, the counting measure characterizes the distance to a product state with a number and even permits modifications when we apply the mean field limit. Hence, ω^φ is more significant and softer than the L^2 -norm. For completeness, we add the computation of the ratio of bad particles of an almost product state which we described in (9). The steps are similar to the calculation we do in (12).

$$\begin{aligned}
\omega^\varphi &= \langle \langle \Psi_N | q_1^\varphi | \Psi_N \rangle \rangle = 1 - \langle \langle \Psi_N | p_1^\varphi | \Psi_N \rangle \rangle \\
&= 1 - \frac{\binom{N-1}{n}}{\binom{N}{n}} = \frac{n}{N} \tag{19}
\end{aligned}$$

In order to emphasize it again, an almost product state has the physical property that most of the bosons are uncorrelated and therefore are in our consideration in identical one-particle states. The correlated particles destroy the product structure which leads in L^2 -norm to the statement, that an almost product state can never behave like a product state. Whereas, the effect with respect to the counting measure is in the mean field limit not of great importance, i.e. if we look from a long way off, the almost product state has the same properties as a product state.

1.5 An alternative counting operator

As a remark, we introduce another notation representing an operator which counts the number of bad particles and therefore is equivalent to the used q_1^φ . First of all, we define

$$P_n^\varphi = \left(\prod_{j=1}^n q_j^\varphi \cdot \prod_{j=n+1}^N p_j^\varphi \right)_{sym.} \tag{20}$$

where *sym.* again stands for symmetric, replacing a sum of $\binom{N}{n}$ terms in order to ensure that every combination of n bad particles out of the N particles x_1, \dots, x_N appears. In addition, we can show that P_n^φ is a projector. Therefore we compute the product of two different operators.

$$\begin{aligned} P_n^\varphi P_m^\varphi &= \left(\prod_{j=1}^n q_j^\varphi \cdot \prod_{k=n+1}^N p_k^\varphi \right)_{sym.} \cdot \left(\prod_{j=1}^m q_j^\varphi \cdot \prod_{k=m+1}^N p_k^\varphi \right)_{sym.} \\ &= \left(\prod_{j=1}^n q_j^\varphi \cdot \prod_{k=n+1}^N p_k^\varphi \right)_{sym.} \delta_{nm} = P_n^\varphi \delta_{nm} \end{aligned} \quad (21)$$

Since only the diagonal terms in the symmetrization survive due to the projection properties of p_i^φ and q_i^φ . Furthermore, the sum of P_n^φ over all numbers of bad particles from 0 to N has to be the identity on $L^2(\mathbb{R}^{3N})$. In order to show this, we write

$$\begin{aligned} \sum_{n=0}^N P_n^\varphi &= \sum_{n=0}^N \left(\prod_{j=0}^n q_j \prod_{k=n+1}^N p_k^\varphi \right)_{sym.} \\ &= \sum_{n=0}^{N-1} \left(\prod_{j=0}^n q_j \prod_{k=n+1}^{N-1} p_k^\varphi \right)_{sym.} (q_N + p_N^\varphi) \\ &= \dots = \prod_{j=1}^N (q_j + p_j^\varphi) = \prod_{j=1}^N \mathbb{1}_j = \bigotimes_{j=1}^N \mathbb{1}_j = \mathbb{1}_{\mathbb{R}^{3N}} \end{aligned} \quad (22)$$

Here, $\mathbb{1}_j$ represents the identity for the j -th particle and $\mathbb{1}_{\mathbb{R}^{3N}}$ expresses the identity for the whole system. Besides, $\bigotimes_{j=1}^N \mathbb{1}_j$ states the direct product of all one-particle identities. Moreover, P_n^φ acting on an N -particle state gives a one if exactly n particles are bad, else a zero.

By the way, if there are any mixed states which are neither good nor bad, the operator just gives a product of all the different weights of the bad state.

Moreover we multiply P_n^φ with the weight $\frac{n}{N}$ and then sum over all possible numbers of bad particles, i.e. from 0 to N . Then we gain an operator giving the relative number of bad bosons of an N -particle state. To conclude, the created operator reads as

$$\hat{n} = \sum_{n=0}^N \frac{n}{N} P_n^\varphi, \quad (23)$$

which is sandwiched by an N -particle state the same as

$$\omega^\varphi = \langle \langle \Psi_N | q_1^\varphi | \Psi_N \rangle \rangle = \left\langle \left\langle \Psi_N \left| \sum_{n=0}^N \frac{n}{N} P_n^\varphi \right| \Psi_N \right\rangle \right\rangle, \quad (24)$$

In order to prove this identity (24), we multiply both operators with P_k^φ , moreover we use $\langle \langle \Phi | q_i^\varphi | \Phi \rangle \rangle = \frac{1}{N} \sum_{j=1}^N \langle \langle \Phi | q_j^\varphi | \Phi \rangle \rangle$, which is only true since we act on symmetric wave functions $\Phi \in L^2(\mathbb{R}^{3N})$. Therefore we have to show that the identity

$$\frac{1}{N} \sum_{j=1}^N q_j^\varphi P_k^\varphi = \frac{k}{N} P_k^\varphi \quad (25)$$

holds. The equation above is valid because P_k^φ consists of k different q_l^φ . Therefore the sum gives k times a 1 since $(q_l^\varphi)^2 = q_l^\varphi$ and $N-k$ times a 0 since $q_l^\varphi p_l^\varphi = 0$ holds true, due to the projector properties. Consequently the equality (25) follows. On the righthand side, we receive according to (21)

$$\sum_{n=0}^N \frac{n}{N} P_n^\varphi P_k^\varphi = \frac{k}{N} P_k^\varphi. \quad (26)$$

The sum is killed as a consequence of the projector property of the q_l^φ and p_l^φ . Finally, with (23) we gain an alternative operator which produces the ratio of bad particles.

1.6 Common ground of $\mu^{\Psi_N^t}$ and ω^{φ^t}

All statements given up to this point are valid for all times t . So far, we have neglected the time dependence in our consideration, in the following, we add the time in our notation. Moreover, the dynamics of Ψ_N^t and φ^t are given by the Schrödinger equation and Hartree equation respectively which we discuss in section 3.1 and 3.2. In order to show the common ground of $\mu^{\Psi_N^t}$ and ω^{φ^t} , we prove the following lemma.

Lemma:

The reduced one-particle density matrix converges in operator norm in the mean field limit to the pure state given by φ^t for all times t if and only if the counting measure converges to zero at this point of time.

Proof:

We show this with the following equality

$$\begin{aligned} 0 &= \left\langle \varphi^t \left| \left(|\varphi^t\rangle \langle \varphi^t| - \lim_{N \rightarrow \infty} \mu^{\Psi_N^t} \right)_{op} \right| \varphi^t \right\rangle \\ &= 1 - \lim_{N \rightarrow \infty} \left\langle \varphi^t \left| \mu^{\Psi_N^t} \right| \varphi^t \right\rangle \\ &= \langle \langle \Psi_N^t | \Psi_N^t \rangle \rangle - \lim_{N \rightarrow \infty} \langle \langle \Psi_N^t | \varphi^t \rangle \langle \varphi^t | \Psi_N^t \rangle \rangle \\ &= \lim_{N \rightarrow \infty} \langle \langle \Psi_N^t | 1 - p_1^{\varphi^t} | \Psi_N^t \rangle \rangle \\ &= \lim_{N \rightarrow \infty} \langle \langle \Psi_N^t | q_1^{\varphi^t} | \Psi_N^t \rangle \rangle \\ &= \lim_{N \rightarrow \infty} \omega^{\varphi^t} = 0 \end{aligned} \quad (27)$$

which can be read in both directions.

Finally, to close the circle, we give a heuristic argument in order to show that

$$\lim_{N \rightarrow \infty} \omega^{\varphi^t} = \lim_{N \rightarrow \infty} \langle \langle \Psi_N^t | q_1^{\varphi^t} | \Psi_N^t \rangle \rangle = 0 \quad (28)$$

leads to the statement that Ψ_N^t is an almost product state. For convenience, we write in the following,

$$0 \approx \langle \langle \Psi_N^t | q_1^{\varphi^t} | \Psi_N^t \rangle \rangle = \langle \langle \Psi_N^t | \Psi_N^t - p_1^{\varphi^t} \Psi_N^t \rangle \rangle. \quad (29)$$

Consequently, the expression (28) corresponds to

$$p_1^{\varphi^t} \Psi_N^t \approx \Psi_N^t \quad (30)$$

which is defined as

$$\begin{aligned} p_1^{\varphi^t} \Psi_N^t(x_1, \dots, x_N) &= p_k^{\varphi^t} \Psi_N^t(x_1, \dots, x_k, \dots, x_N) \\ &= \varphi^t(x_k) \int \varphi^{t*}(x_k) \Psi_N^t(x_1, \dots, x_k, \dots, x_N) dx_k \approx \Psi_N^t(x_1, \dots, x_k, \dots, x_N). \end{aligned} \quad (31)$$

Here, the first equivalence holds true since Ψ_N^t is symmetric and $k \in \{1, \dots, N\}$. Furthermore, the projector acts on the N-particle state by replacing the one-particle state of particle x_k with φ^t . Finally, we arrive at an N-particle state which is approximately identical to Ψ_N^t . Consequently, most of the particles in this state behave well and are in the one-particle state φ^t which we want. In other words, a small amount of bosons which can be neglected in the mean field limit, is in some other state.

Next, we consider the case that there are $n \ll N$ bad particles in our bosonic system. Without loss of generality, we assume that these bosons are in some state which is orthogonal to φ^t . Therefore, we end up with an N-particle state which looks as described in (9) while (8) holds true. Since Ψ_N^t is invariant with respect to particle exchange, only n summands out of $\binom{N}{n}$ disappear when $p_1^{\varphi^t}$ acts on Ψ_N^t . That is the reason why $p_1^{\varphi^t} \Psi_N^t$ and Ψ_N^t do not differ from each other in a rough way. Consequently, (30) holds true for large N.

To sum up, if we take (28) for granted, then Ψ_N^t can be written as an almost product state.

To conclude, in this part, we declare the connections between an almost product state Ψ_N^t , the reduced one-particle density matrix $\mu^{\Psi_N^t}$ and the counting measure ω^{φ^t} . The final goal is to prove that an initial almost product state keeps its structure for all finite times t. The most obvious way to show this is the analysis of the time evolution of the ratio of bad particles. Assuming that the number of bad particles is small in the initial state and vanishes in the mean field limit, we demonstrate in the following that the same holds true for all finite times. Moreover, we use the equivalences (2) illustrated in this section in order to arrive at the aim described above. To sum up, we confirm that

$$\begin{array}{ccc} \Psi_N^0 & & \Psi_N^t \\ \text{almost product state} & & \text{almost product state} \\ \Downarrow & & \Downarrow \\ \mu^{\Psi^0} \xrightarrow{N \rightarrow \infty} |\varphi^0\rangle \langle \varphi^0| & & \mu^{\Psi^t} \xrightarrow{N \rightarrow \infty} |\varphi^t\rangle \langle \varphi^t| \\ \Downarrow & & \Downarrow \\ \omega^{\varphi^0} \xrightarrow{N \rightarrow \infty} 0 & \Leftrightarrow & \omega^{\varphi^t} \xrightarrow{N \rightarrow \infty} 0 \end{array}$$

is valid for all finite times. As drawn above, we connect the initial properties with the characteristics at some finite time t via the ratio of bad particles. Consequently, it is enough to give an upper bound for the ratio of bad particles which converges in the mean field limit to 0.

With respect to this objective, we take advantage of the Grönwall Lemma which we present in the following. For reasons of completeness, we also add one of its proofs.

2 The Grönwall Lemma

Lemma:

Let $a(t)$ and $b(t)$ be non-negative continuous functions defined on an interval $[0, T]$ with $T > 0$. Let $f(t)$ be a non-negative continuous differentiable function on $[0, T]$ with

$$f'(t) \leq a(t)f(t) + b(t) \quad \forall t \in [0, T] \quad (32)$$

Then

$$f(t) \leq e^{\int_0^t a(s) ds} \left(f(0) + \int_0^t b(s) e^{-\int_0^s a(\tau) d\tau} ds \right) \quad (33)$$

holds true for all $t \in [0, T]$

Proof:

Let $g(t) \in C^1([0, T])$ be such that

$$g'(t) = a(t)g(t) + b(t) \quad (34)$$

This is an ordinary differential equation which can be solved uniquely on $[0, T]$. Accordingly, the solution of this initial value problem reads as

$$g(t) = e^{\int_0^t a(s) ds} \left(g(0) + \int_0^t b(s) e^{-\int_0^s a(\tau) d\tau} ds \right). \quad (35)$$

Moreover, we take for granted that

$$\begin{aligned} f(0) &\leq g(0) \\ \text{we shall show, that } f(t) &\leq g(t) \end{aligned} \quad (36)$$

holds true for all $t \in [0, T]$.

Assume for contradiction, there is a $t_1 \in (0, T)$ such that $f(t_1) > g(t_1)$. Since f and g are continuous functions on $[0, T]$, the intermediate value theorem assures that there is a $t_0 \in (0, T)$ where we define t_0 as $t_0 := \min \{t \in (0, t_1) \mid g(t) = f(t)\}$.

Now, we deal with the function

$$\begin{aligned} F : [0, T] &\rightarrow \mathbb{R} \\ t &\mapsto F(t) = g(t) - f(t) \end{aligned} \quad (37)$$

We know from above that $F(0) \geq 0$ and $F(t_0) = 0$ holds. Because of the mean value theorem for continuous functions, there exists a $\tilde{t} \in (0, t_0)$ such that

$$F'(\tilde{t}) = \frac{F(t_0) - F(0)}{t_0 - 0} = -\frac{F(0)}{t_0} \leq 0 \quad (38)$$

and therefore

$$g'(\tilde{t}) - f'(\tilde{t}) \leq 0 \quad (39)$$

Moreover, from the definition and given constraints we can deduce

$$a(\tilde{t}) \left(g(\tilde{t}) - f(\tilde{t}) \right) \leq g'(\tilde{t}) - f'(\tilde{t}) \leq 0 \quad (40)$$

and as a consequence we gain

$$g(\tilde{t}) \leq f(\tilde{t}). \quad (41)$$

However, this contradicts to the definition of t_0 to be the smallest positive value apart from 0 such that the functional values of f and g agree with each other. That is the reason, why $f(t) \leq g(t)$ holds for all $t \in [0, T]$.

Finally

$$f(t) \leq e^{\int_0^t a(s) ds} \left(f(0) + \int_0^t b(s) e^{-\int_0^s a(\tau) d\tau} ds \right) \quad (42)$$

is bounded from above. In our later description, t is the time parameter which can be stretched arbitrarily, since T is not a fixed value. Therefore we should ask, under which conditions is the upper bound in (42) reasonable, especially when T goes to infinity. Since $f(t)$ is a non-negative function and in order to get a useful limit from above, we have to exclude the fact that it blows up to infinity. Consequently, we have to demand the functions $a(t)$ and $b(t)$ to be integrable on the interval $[0, \infty)$.

With a view to this lemma, we formulate its property in this way. Under the condition that any function whose derivative can be estimated with the function itself from above, the Grönwall Lemma allows us to restrict the function from above via an initial value and any smooth functions.

In the treated case, we use it as follows. If we can show that the time derivative of the ratio of bad particles ω^{φ^t} has a reasonable upper bound depending in an affine way on ω^{φ^t} , then as a consequence of the Grönwall Lemma, we will get a limit from above for ω^{φ^t} .

3 The Bosonic System

We are now at the point where we have to describe the bosonic N -particle system in detail.

3.1 The Hamiltonian of the system

It was already mentioned that due to the bosons, the N -particle state $\Psi_N(x_1, \dots, x_N)$, normalized to one, is symmetric under the interchange of particles. Moreover each boson moves with a kinetic energy in a perhaps time dependent potential A^t . In addition, we allow pair interaction, whereas we neglect for simplicity the interaction of three or more particles. Besides, the structure of the result will not change, if we also accept interaction of higher order. To conclude, the Hamiltonian

$$H_N = \sum_{j=1}^N (-\Delta_j) + \sum_{j=1}^N A^t(x_j) + \sum_{1 \leq j < k \leq N} V_N(x_j - x_k) \quad (43)$$

describes the N -particle system, where we set $\frac{\hbar^2}{2m}$ to one.

We have to consider the real valued interaction V_N , i.e. a physical correct choice of the order due to the number of particles, as well as its domain. Note that the order of the kinetic energy as well as the order of the potential are fixed to the number of particles N according to expression (43). We can imagine different possibilities of the sharing out of the energy in the system. If the kinetic term dominates the energy, we can treat the bosons as free particles moving in a potential. This means, the particles do not feel each other. However, if the interaction energy is much larger than the kinetic energy of the bosons, it follows that we can interpret the system containing just resting particles as a result of the interaction. We want to have a balanced and therefore a physical interesting system. Here, we mean balanced in the sense of the order of the kinetic term equals the order of the interaction. As a consequence we need to scale V_N with $\frac{1}{N}$ to reach a final order of N in the Hamiltonian

$$V_N(x) = \frac{1}{N}v(x). \quad (44)$$

The reason for that is, that $\sum_{1 \leq j < k \leq N} V_N(x_j - x_k)$ consists of $\binom{N}{2}$ terms, which is of order N^2 .

Moreover, another heuristic argument for the scaling factor in (44) is the following. We assume that the distribution of particles in a volume element in our bosonic system is homogeneous and proportional to N . Therefore, if the number of particles grows, also the strength of the interaction increases linear in N in the volume element. In order to keep the strength of the pair interaction independent from the particle number, we rescale the interaction term with $\frac{1}{N}$.

Besides, for some reasons which become clear later, we also take for granted, that the interaction $V_N, v \in L^{2r}(\mathbb{R}^{3N})$ with $1 \leq r \leq \infty$ arbitrary, coming from an Hölder estimate.

Similarly, the time dependent N -particle state Ψ_N^t satisfies the Schrödinger equation, with the Hamiltonian from (43)

$$i\partial_t \Psi_N^t = H_N \Psi_N^t. \quad (45)$$

In principle, we are done and can stop here, just at this point. The reason for that is, given Ψ_N at time $t = 0$, we can determine Ψ_N^t via this partial differential equation. Afterwards, we count the bad particles at time t in Ψ_N^t by computing

$$\omega^{\varphi^t} = \left\langle \left\langle \Psi_N^t \left| q_1^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \quad (46)$$

and this result is what we want. It sounds easy, however, the computation stretches to infinity, because we are studying systems with a number of particles in the range of $10^4 - 10^7$ (cf. [2] p. 812), converging in the mean field limit to infinity.

That is the reason, why we have to follow another strategy. As already mentioned, we want to make use of the Grönwall lemma. Therefore we have to estimate the absolute value of the time derivative of ω^{φ^t} and hence the derivative of q^{φ^t} .

3.2 The Hartree equation of one single boson

First of all, let us have a look on the behavior of one single particle in the mean field of all the $N-1$ others. Therefore, we make an intuitive ansatz. We can be sure that a particle has kinetic energy, as well as it moves in the external potential. In addition we also have to take into account the pair interaction with the remaining other particles, i.e. a test particle moves in a potential caused by the other bosons. To conclude, our ansatz for the Schrödinger equation of one particle in the mean field of all the others reads as

$$i\partial_t\varphi^t = (-\Delta + A^t + (N-1)W)\varphi^t \quad (47)$$

which is the macroscopic consideration of our system. We have to think about the interaction term W based on the pair interaction. We know, if two particles x and y interact with each other, we get a term $V_N(x-y)$ where V_N is the same interaction which we already used in (43). However, if m particles interact with x , we obtain $\sum_{j=1}^m V_N(x-y_j)$. Moreover, in the case that more than one particle is localized near the position y_j we have to introduce another function, in other words a weight $Z(y_j)$ giving the number of particles around the place y_j . For convenience, we can normalize the weight to 1. Therefore we receive the formula

$$\sum_{j=1}^m \frac{Z(y_j)}{N} V_N(x-y_j). \quad (48)$$

The discrete function $\frac{Z(y_j)}{N}$ corresponds to the empirical density, expressing the distribution of N particles in the position space \mathbb{R}^3 around our test particle x . For large N , especially N going to infinity, the sum above transforms into an integral and $\frac{Z(y_j)}{N}$ changes into a continuous empirical, time dependent, density $\rho^t(y)$. Because of this limit, the interaction term in (47) can be written as

$$W = V_N^{\rho^t} = \int \rho^t(y) V_N(x-y) dy. \quad (49)$$

Finally, we have to clarify the structure of $\rho^t(y)$. We show next that

$$\rho^t(x) = \rho_{th}^t(x) = |\varphi^t(x)|^2 \quad (50)$$

where $\rho_{th}^t(x)$ means the theoretical density in \mathbb{R}^3 . In general, this expression describes a probability distribution of the places of the particles in \mathbb{R}^3 . Indeed, it is a calculated theoretical characteristic, which is accompanied by the expectation value and the standard deviation. Let ρ^t be a probability distribution, then $dp = \rho^t dV$ is the probability to find a particle in an explicit, infinitesimal volume dV at the place x . Let us stretch this statement to k particles out of N are at the position x and we arrive at the Binomial distribution $B(N, k, p) = \binom{N}{k} p^k q^{N-k}$, where p is the probability that one particle is at x and $q := 1 - p$. The expectation value can be computed as Np as well as the standard deviation $\sigma = \sqrt{Npq}$, which figures out the average deviation of the expectation value. For large N , we can be sure according to the law of large numbers that the ascertainable number of particles being located at the point x , $n(x)$ fulfills

$$|Np - n(x)| < \sqrt{N}. \quad (51)$$

Relatively, the experimental measurable value $\frac{n(x)}{N}$ has to converge to p because $\frac{1}{\sqrt{N}}$ converges to 0 for N going to infinity.

Let us build a bridge from the theoretical probability distribution to the experimental confirmable empirical distribution. The difference between both

$$|\rho_{th}^t - \rho_{emp}^t| \in \mathcal{O}(\sqrt{N}) \quad (52)$$

has to be at most of order \sqrt{N} as studied above. Since the Hartree equation works in the macroscopic system, we need a particle distribution which is measurable in the experiment and not theoretically predicted. Therefore we plug this result into (49) and receive

$$V_N^{\rho^t} = \int \rho_{emp}^t(y) V_N(x-y) dy + \int \mathcal{O}(\sqrt{N}) V_N(x-y) dy. \quad (53)$$

To come to an end, for the reason that we consider the mean field limit and due to the fact that $V_N \in \mathcal{O}(\frac{1}{N})$ holds, the second summand converges like $\frac{1}{\sqrt{N}}$ to 0.

In order to go from the probability to the empirical density we have to pay a price, a term of order $\frac{1}{\sqrt{N}}$ which can be neglected for sufficient large N. Finally (47) reads as

$$\begin{aligned} i\partial_t \varphi^t &= h_N^{mf} \varphi^t \\ i\partial_t \varphi^t &= \left(-\Delta + A^t + (N-1) (V_N * |\varphi^t|^2) \right) \varphi^t \end{aligned} \quad (54)$$

which is called the Hartree equation and where we have to emphasize that $|\varphi^t|^2$ is an empirical density if and only if we treat systems with big particle numbers. For that reason, this ansatz of the one-particle Schrödinger equation just makes sense, if and only if we analyze many particle systems. Notice, $*$ denotes a convolution and is defined as $(f * g)(x) = \int f(y)g(x-y)dx$.

By the way, it seems surprising that the Hartree equation is nonlinear with respect to the one-particle state. It is the macroscopic description of one single particle in the bosonic system, whereas the Schrödinger equation determines the dynamics of the whole system and is indeed linear. Therefore, one could argue, that there are some inconsistencies.

In order to explain this issue, we have to look at the general picture, i.e. the equality as well as the initial wave function. For sure, the Schrödinger equation itself is linear, however, we take for granted that the initial N-particle state has (almost) product structure and is therefore nonlinear with respect to the one-particle state. Moreover, the Hartree equation is nonlinear in φ while its initial condition is the one-particle state itself.

The point is, we have to prove that this heuristic discussion of the Hartree equation can be done rigorously, i.e. the considered bosonic system really behaves in that way. In section 3.4.4 we go into details and show that the interaction term is chosen right.

3.3 Fair comments on the literature

In the literature there is often claimed that the Hartree equation can be derived from varying the energy $\langle \langle \Psi_N | H_N | \Psi_N \rangle \rangle$ with respect to a single one-particle function φ under the condition that this state is normalized to one. Computationally, we get the right equation. The interaction term results with the correct structure as well as the prefactor corresponds to our preliminary consideration.

We present two short and very important reasons, why this computation is right, however, it does not explain the physics which is behind.

To start with, the computation holds for every particle number N, especially also for less N. As already mentioned, in the discussion above, in order to make sense, we intend the interaction term to be weighted with the empirical density - not the probability density. In the deviations in the literature there is never lost a word on “N going to infinity”, which is an important point to be taken into account.

To be continued, there is an unknown input, the N-particle state Ψ_N . In the literature, there is assumed, that for all times t , Ψ_N can be expressed by a product state. Why can we take exactly this structure for granted? Who tells us that this ansatz corresponds to the time evolution and therefore to the physics in our system? For the sake of simplicity, we can demand such a Ψ_N , nevertheless, in order to keep generality there is no argument, why nature should behave like this. It is a crucial hypothesis to demand that initial states which have product structure remain for all times states with product form, too. Due to the fact that we have correlation and interactions, it is quite courage to claim this out of the blue.

In the following addition, we show that in general we cannot take for granted that an initial product state of an arbitrary system keeps its structure at least for all finite times t and for all particle numbers N . For that reason, we consider a three dimensional system consisting of two identical free bosons which interact via Coulomb interaction and which are located at x_1 and x_2 . Moreover, we assume that the initial two-particle eigenstate has product structure, i.e. $\Psi^0(x_1, x_2) = \varphi^0(x_1) \cdot \varphi^0(x_2)$, where φ represents an in $L^2(\mathbb{R}^3)$ -norm normalized one-particle state. For convenience, we multiply the Coulomb interaction with a factor of 2. Consequently, if we take for granted that Ψ^t keeps its product structure for finite t , the time-dependent Schrödinger equation reads as

$$\left(-\Delta_{x_1} - \Delta_{x_2} + \frac{2}{|x_1 - x_2|}\right) \varphi^t(x_1)\varphi^t(x_2) = i\partial_t(\varphi^t(x_1)\varphi^t(x_2)), \quad (55)$$

reordering yields to

$$\left[\left(-\Delta_{x_1} + \frac{1}{|x_1 - x_2|}\right) \varphi^t(x_1) - i\dot{\varphi}^t(x_1)\right] \varphi^t(x_2) = - \left[\left(-\Delta_{x_2} + \frac{1}{|x_2 - x_1|}\right) \varphi^t(x_2) - i\dot{\varphi}^t(x_2)\right] \varphi^t(x_1) \quad (56)$$

which can also be written as

$$-\frac{\varphi^t(x_1)}{\varphi^t(x_2)} = \frac{\left(-\Delta_{x_1} + \frac{1}{|x_1 - x_2|}\right) \varphi^t(x_1) - i\dot{\varphi}^t(x_1)}{\left(-\Delta_{x_2} + \frac{1}{|x_2 - x_1|}\right) \varphi^t(x_2) - i\dot{\varphi}^t(x_2)} \quad (57)$$

This expression has to hold true for all $x_1, x_2 \in \mathbb{R}^3$ and therefore also for the limit $x_1 \rightarrow x_2$, which exists, since $\varphi(x_1)$ and $\varphi(x_2)$ exist. Nevertheless, for small distances the Coulomb interaction term dominates the right hand side of (57). In this case, we arrive at

$$-\frac{\varphi^t(x_1)}{\varphi^t(x_2)} = \frac{\varphi^t(x_1)}{\varphi^t(x_2)}. \quad (58)$$

From this result, we infer that $\varphi^t(x_1) = 0 \forall x_1 \in \mathbb{R}^3$ and therefore $\varphi^t \equiv 0$. However, this contradicts to the assumption $\|\varphi^t\|_2 = 1$.

To conclude, provided that the initial state of a system is a product state, the generalization for small particle numbers to finite times usually fails. Consequently, the wave function of the whole system cannot be written as a product state.

In fact, there are two things to show, on the one hand the validity of the Hartree equation and on the other hand the conservation of the product structure of the N -particle state for all times t and huge N . We will show the former by the by, whereas the latter is really hard work.

In addition, what do we mean by varying $\langle\langle \Psi_N | H_N | \Psi_N \rangle\rangle$? To be more concrete, let us better write varying $\langle\langle \prod_{j=1}^N \varphi_j | H_N | \prod_{j=1}^N \varphi_j \rangle\rangle$. This means, that we are looking for extreme values of this scalar product with respect to φ . Since our system is stable, we know that the energy has to be bounded from below, despite, the energy has no upper limit. Indeed, a physical system looks always for the lowest possible energy state and therefore, we can find a minimum, the ground state energy of the N particles called $E_{N,G}$, with the corresponding ground state φ_G . Moreover, we use the mean field Hamiltonian as defined in (54).

In this way, we just arrive at one equation

$$h_N^{mf} \varphi_G = \frac{E_{N,G}}{N} \varphi_G \quad (59)$$

where $\frac{E_{N,G}}{N}$ denotes the energy of every single particle, since we consider bosons and φ_G the ground state. On the one hand, since h_N^{mf} is for sure not a projection, it is impossible to infer a unique operator with the help of one single eigenstate and its corresponding eigenvalue. On the other hand, we cannot deduce any advantage for the determination of the dynamic of φ , unless, we compute every single eigenstate ϕ and eigenvalue e of

$$h_N^{mf} \phi = e\phi. \quad (60)$$

We are not going to proceed in this way, because we gain afterwards with less effort a more general result, which also includes this topic.

3.4 The upper bound of the relative number of bad particles

After having explained the physical aspects, we will continue with some calculation intending to use Grönwall's Lemma at the end. For the sake of simplicity, we abstain at the moment from detailed estimates which we use in the following. Here, we just want to present the pursued idea for the assessments. Nevertheless we add them in section 3.4.5.

3.4.1 The time derivative of ω^{φ^t}

Now we are studying the behavior of the time derivative of the number of bad particles at any finite time t . As a consequence of the symmetry of $\Psi_N^t(x_1, \dots, x_N)$ due to particle interchange, we are free to choose one particle, e.g. we take x_1 . Moreover, we use the Schrödinger equation (45) to express the time derivative of Ψ_N^t .

$$\begin{aligned} \dot{\omega}^{\varphi^t} &= \left(\left\langle \left\langle \Psi_N^t \left| \dot{q}_1^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right) \\ &= \left\langle \left\langle \dot{\Psi}_N^t \left| q_1^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle + \left\langle \left\langle \Psi_N^t \left| \dot{q}_1^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle + \left\langle \left\langle \Psi_N^t \left| q_1^{\varphi^t} \right| \dot{\Psi}_N^t \right\rangle \right\rangle \\ &= i \left\langle \left\langle \Psi_N^t \left| H_N q_1^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle - i \left\langle \left\langle \Psi_N^t \left| q_1^{\varphi^t} H_N \right| \Psi_N^t \right\rangle \right\rangle + \left\langle \left\langle \Psi_N^t \left| \dot{q}_1^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \\ &= i \left\langle \left\langle \Psi_N^t \left| [H_N, q_1^{\varphi^t}] \right| \Psi_N^t \right\rangle \right\rangle + \left\langle \left\langle \Psi_N^t \left| \dot{q}_1^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \end{aligned} \quad (61)$$

Recall, that $[A, B] = AB - BA$ denotes the commutator, moreover, H_N is the N-particle Hamiltonian. In the following, the Hartree equation takes on the task of the Schrödinger equation in the computation above.

$$\begin{aligned} \dot{q}_i^{\varphi^t} &= \left(1 - p_i^{\varphi^t} \right) \dot{\varphi}_i^t = - \left(|\varphi_i^t\rangle \langle \varphi_i^t| + |\varphi_i^t\rangle \langle \dot{\varphi}_i^t| \right) \\ &= i \left(h_N^{mf}(x_i) |\varphi_i^t\rangle \langle \varphi_i^t| - |\varphi_i^t\rangle \langle \varphi_i^t| h_N^{mf}(x_i) \right) \\ &= i \left(h_N^{mf}(x_i) p_i^{\varphi^t} - p_i^{\varphi^t} h_N^{mf}(x_i) \right) \\ &= i \left[h_N^{mf}(x_i), p_i^{\varphi^t} \right] = -i \left[h_N^{mf}(x_i), 1 - p_i^{\varphi^t} \right] = -i \left[h_N^{mf}(x_i), q_i^{\varphi^t} \right] \end{aligned} \quad (62)$$

To sum up, we get for the time derivative of ω^{φ^t}

$$\dot{\omega}^{\varphi^t} = i \left\langle \left\langle \Psi_N^t \left| [H_N - h_N^{mf}(x_1), q_1^{\varphi^t}] \right| \Psi_N^t \right\rangle \right\rangle \quad (63)$$

In detail, the projector $q_1^{\varphi^t}$ acts only on functions depending on the variable x_1 . Therefore with regard to (62), also h_N^{mf} just depends on the x_1 particle. In general we receive

$$\begin{aligned} \dot{\omega}^{\varphi^t} = i \left\langle \left\langle \Psi_N^t \left| \left[\left(\sum_{k=1}^N (-\Delta_k) + \sum_{k=1}^N A^t(x_k) + \sum_{1 \leq k < l \leq N} V_N(x_l - x_k) \right) \right. \right. \right. \\ \left. \left. \left. - \left(-\Delta_1 + A^t(x_1) + (N-1) \left(V_N * |\varphi^t|^2 \right)(x_1) \right), q_1^{\varphi^t} \right] \right| \Psi_N^t \right\rangle \right\rangle. \end{aligned} \quad (64)$$

Since for arbitrary projectors T and S and for all $1 \leq i, j \leq N$ with $i \neq j$

$$[T(x_i), S(x_j)] = 0 \quad (65)$$

holds, only the x_1 dependent terms in H_N do not commute in (63). Besides, the interaction term consists of the sum over all other remaining particles x_2, \dots, x_N . We apply the argument of symmetry and arrive at $N-1$ times the interaction of one arbitrarily labeled particle, say x_2 with x_1 . That is the reason, why the time derivative of ω^{φ^t} simplifies to

$$\begin{aligned} \dot{\omega}^{\varphi^t} = i \left\langle \left\langle \Psi_N^t \left| \left[\left(-\Delta_1 + A^t(x_1) + (N-1) V_N(x_1 - x_2) \right) \right. \right. \right. \\ \left. \left. \left. - \left(-\Delta_1 + A^t(x_1) + (N-1) \left(V_N * |\varphi^t|^2 \right)(x_1) \right), q_1^{\varphi^t} \right] \right| \Psi_N^t \right\rangle \right\rangle \\ = i(N-1) \left\langle \left\langle \Psi_N^t \left| \left[V_N(x_1 - x_2) - \left(V_N * |\varphi^t|^2 \right)(x_1), q_1^{\varphi^t} \right] \right| \Psi_N^t \right\rangle \right\rangle \end{aligned} \quad (66)$$

We recognize that the change in time of the number of bad particles is based on the difference of the real interaction due to the Hamiltonian H_N and the assumed interaction term with respect to the Hartree equation. To repeat, if we can show, that (66) converges to zero for N going to infinity, then we can be sure that the interaction term in the Hartree equation (54) is chosen correctly.

3.4.2 Insertion of identities

It seems that we are stuck up a blind alley, because we are not aware of any details of Ψ_N^t . The only known property connected with the initial (almost) product state Ψ_N^0 is that ω^{φ^0} converges for $N \rightarrow \infty$ to 0 which is equivalent to $\mu^{\Psi_N^0} \xrightarrow{N \rightarrow \infty} |\varphi^0\rangle \langle \varphi^0|$ in operator norm. Consequently, we have no idea how Ψ_N^t acts on the commutator in (66). Besides, we are familiar to the action of $p_i^{\varphi^t}$ and $q_i^{\varphi^t}$ to the interaction terms. As a consequence, we insert at the right position further identities $1 = p_i^{\varphi^t} + q_i^{\varphi^t}$ which of course do not change the equality (66), but make life easier. By the way, for the sake of clarity we sum up the difference of the interactions in a function

$$f(x_1, x_2) = V_N(x_1 - x_2) - \left(V_N * |\varphi^t|^2 \right)(x_1). \quad (67)$$

From the relation (66) we gain

$$\begin{aligned} \left| \dot{\omega}^{\varphi^t} \right| = (N-1) \left| \left\langle \left\langle \Psi_N^t \left| f(x_1, x_2) q_1^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle - \left\langle \left\langle \Psi_N^t \left| q_1^{\varphi^t} f(x_1, x_2) \right| \Psi_N^t \right\rangle \right\rangle \right| \\ = (N-1) \left| \left\langle \left\langle \Psi_N^t \left| (p_1^{\varphi^t} + q_1^{\varphi^t})(p_2^{\varphi^t} + q_2^{\varphi^t}) f(x_1, x_2) q_1^{\varphi^t} (p_2^{\varphi^t} + q_2^{\varphi^t}) \right| \Psi_N^t \right\rangle \right\rangle \right. \\ \left. - \left\langle \left\langle \Psi_N^t \left| (p_2^{\varphi^t} + q_2^{\varphi^t}) q_1^{\varphi^t} f(x_1, x_2) (p_1^{\varphi^t} + q_1^{\varphi^t})(p_2^{\varphi^t} + q_2^{\varphi^t}) \right| \Psi_N^t \right\rangle \right\rangle \right| \end{aligned} \quad (68)$$

At first glance, it seems that we created 16 terms from two terms, but looking at it again, most of the terms cancel out and we keep three different terms with their complex conjugate. In detail, since we drop the function f in the middle for a moment, we have for the sign

“+”	(i) $p_1^{\varphi^t} p_2^{\varphi^t}$ $q_1^{\varphi^t} p_2^{\varphi^t}$ (ii) $p_1^{\varphi^t} p_2^{\varphi^t}$ $q_1^{\varphi^t} q_2^{\varphi^t}$ (iii) $p_1^{\varphi^t} q_2^{\varphi^t}$ $q_1^{\varphi^t} p_2^{\varphi^t}$ (iv) $p_1^{\varphi^t} q_2^{\varphi^t}$ $q_1^{\varphi^t} q_2^{\varphi^t}$ (v) $q_1^{\varphi^t} p_2^{\varphi^t}$ $q_1^{\varphi^t} p_2^{\varphi^t}$ (vi) $q_1^{\varphi^t} p_2^{\varphi^t}$ $q_1^{\varphi^t} q_2^{\varphi^t}$ (vii) $q_1^{\varphi^t} q_2^{\varphi^t}$ $q_1^{\varphi^t} p_2^{\varphi^t}$ (viii) $q_1^{\varphi^t} q_2^{\varphi^t}$ $q_1^{\varphi^t} q_2^{\varphi^t}$	“-”	(ix) $q_1^{\varphi^t} p_2^{\varphi^t}$ $p_1^{\varphi^t} p_2^{\varphi^t}$ (x) $q_1^{\varphi^t} p_2^{\varphi^t}$ $p_1^{\varphi^t} q_2^{\varphi^t}$ (xi) $q_1^{\varphi^t} p_2^{\varphi^t}$ $q_1^{\varphi^t} p_2^{\varphi^t}$ (xii) $q_1^{\varphi^t} p_2^{\varphi^t}$ $q_1^{\varphi^t} q_2^{\varphi^t}$ (xiii) $q_1^{\varphi^t} q_2^{\varphi^t}$ $p_1^{\varphi^t} p_2^{\varphi^t}$ (xiv) $q_1^{\varphi^t} q_2^{\varphi^t}$ $p_1^{\varphi^t} q_2^{\varphi^t}$ (xv) $q_1^{\varphi^t} q_2^{\varphi^t}$ $q_1^{\varphi^t} p_2^{\varphi^t}$ (xvi) $q_1^{\varphi^t} q_2^{\varphi^t}$ $q_1^{\varphi^t} q_2^{\varphi^t}$.
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Moreover, (v) and (xi), (vi) and (xii), (vii) and (xv), as well as (viii) and (xvi) cancel each other out. Let us have a closer look at the lines (iii) and (x). Here, the interaction term of the mean field Hamiltonian drops out, because it depends only on x_1 and therefore commutes with the projectors $p_2^{\varphi^t}$ and $q_2^{\varphi^t}$. For that reason, the projectors act on each other which gives 0. So the projectors in (iii) and (x) act only on $V(x_1 - x_2)$ which is spherical symmetric. As a consequence, the terms (iii) and (x) cancel each other due to the symmetry of Ψ_N^t .

The remaining three terms are

$$\begin{aligned}
 \text{A) } & p_1^{\varphi^t} p_2^{\varphi^t} f(x_1, x_2) q_1^{\varphi^t} p_2^{\varphi^t} - q_1^{\varphi^t} p_2^{\varphi^t} f(x_1, x_2) p_1^{\varphi^t} p_2^{\varphi^t} \\
 \text{B) } & p_1^{\varphi^t} p_2^{\varphi^t} f(x_1, x_2) q_1^{\varphi^t} q_2^{\varphi^t} - q_1^{\varphi^t} q_2^{\varphi^t} f(x_1, x_2) p_1^{\varphi^t} p_2^{\varphi^t} \\
 \text{C) } & p_1^{\varphi^t} q_2^{\varphi^t} f(x_1, x_2) q_1^{\varphi^t} q_2^{\varphi^t} - q_1^{\varphi^t} q_2^{\varphi^t} f(x_1, x_2) p_1^{\varphi^t} q_2^{\varphi^t}
 \end{aligned}$$

Under the condition that V_N is selfadjoint, also f is selfadjoint and in consequence, by acting on both sides of the terms A), B), C) with Ψ_N^t , we recognize that the differences above are just the complex conjugated of a number subtracted from itself. Since $|z| = |z^*|$ holds for all $z \in \mathbb{C}$ and by using the triangular inequality for the absolute value, (68) simplifies to

$$\begin{aligned}
 |\dot{\omega}^{\varphi^t}| & \leq 2(N-1) \left(\left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} p_2^{\varphi^t} f(x_1, x_2) q_1^{\varphi^t} p_2^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right| \\
 & \quad + \left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} p_2^{\varphi^t} f(x_1, x_2) q_1^{\varphi^t} q_2^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right| \\
 & \quad + \left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} q_2^{\varphi^t} f(x_1, x_2) q_1^{\varphi^t} q_2^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right| \right)
 \end{aligned} \tag{69}$$

and hence,

$$\begin{aligned}
 |\dot{\omega}^{\varphi^t}| & \leq 2(N-1) \left(\left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} p_2^{\varphi^t} \left(V_N(x_1 - x_2) - (V_N * |\varphi^t|^2)(x_1) \right) q_1^{\varphi^t} p_2^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right| \\
 & \quad + \left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} p_2^{\varphi^t} \left(V_N(x_1 - x_2) - (V_N * |\varphi^t|^2)(x_1) \right) q_1^{\varphi^t} q_2^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right| \\
 & \quad + \left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} q_2^{\varphi^t} \left(V_N(x_1 - x_2) - (V_N * |\varphi^t|^2)(x_1) \right) q_1^{\varphi^t} q_2^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right| \right)
 \end{aligned} \tag{70}$$

3.4.3 Estimates

Let us consider the inequality by estimating term by term. Since the prefactor $2(N-1)$ does not influence the computations below, we neglect it at the moment.

Now, we just want to give a general idea of every single assessment for the reason of clearness and therefore the detailed computations follow in section 3.4.5.

For the first term in (70) we get

$$\begin{aligned}
& \left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} p_2^{\varphi^t} \left(V_N(x_1 - x_2) - \left(V_N * |\varphi^t|^2 \right) (x_1) \right) q_1^{\varphi^t} p_2^{\varphi^t} \left| \Psi_N^t \right\rangle \right\rangle \right| \\
&= \left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} \left(p_2^{\varphi^t} V_N(x_1 - x_2) p_2^{\varphi^t} - p_2^{\varphi^t} \left(V_N * |\varphi^t|^2 \right) (x_1) p_2^{\varphi^t} \right) q_1^{\varphi^t} \left| \Psi_N^t \right\rangle \right\rangle \right| \\
&= \left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} \left(p_2^{\varphi^t} \left(V_N * |\varphi^t|^2 \right) (x_1) p_2^{\varphi^t} - p_2^{\varphi^t} \left(V_N * |\varphi^t|^2 \right) (x_1) p_2^{\varphi^t} \right) q_1^{\varphi^t} \left| \Psi_N^t \right\rangle \right\rangle \right| \\
&= 0,
\end{aligned} \tag{71}$$

where we used the identity (85) from below. The first term in (70) is identical to 0 and vanishes independently of N . Furthermore, in section 3.4.4 we concentrate more on this issue.

In order to show the functioning of the estimates, we go on with the third summand of (70). At the end, we want to apply Grönwall's Lemma, therefore we have to proceed in such a way, that $\omega^{\varphi^t} = \left\langle \left\langle \Psi_N^t \left| q^{\varphi^t} \left| \Psi_N^t \right\rangle \right\rangle \right\rangle = \left\| q^{\varphi^t} \Psi_N^t \right\|_2^2$ appears in our estimates.

$$\begin{aligned}
& \left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} q_2^{\varphi^t} \left(V_N(x_1 - x_2) - \left(V_N * |\varphi^t|^2 \right) (x_1) \right) q_1^{\varphi^t} q_2^{\varphi^t} \left| \Psi_N^t \right\rangle \right\rangle \right| \\
&\leq \left\| q_1^{\varphi^t} q_2^{\varphi^t} \Psi_N^t \right\|_2 \left\| \left(V_N(x_1 - x_2) - \left(V_N * |\varphi^t|^2 \right) (x_1) \right) p_1^{\varphi^t} q_2^{\varphi^t} \Psi_N^t \right\|_2 \\
&\leq \left\| q_1^{\varphi^t} \right\|_{op} \left\| q_2^{\varphi^t} \Psi_N^t \right\|_2 \left\| p_1^{\varphi^t} \left(V_N(x_1 - x_2) - \left(V_N * |\varphi^t|^2 \right) (x_1) \right)^2 p_1^{\varphi^t} \right\|_{op}^{\frac{1}{2}} \left\| q_2^{\varphi^t} \Psi_N^t \right\|_2 \\
&\stackrel{(46)}{\leq} 2 \left\| \varphi^t \right\|_{2s} \left\| V_N \right\|_{2r} \omega^{\varphi^t} \\
&\stackrel{(89)}{\leq} 2 \left\| \varphi^t \right\|_{2s} \left\| V_N \right\|_{2r} \omega^{\varphi^t}
\end{aligned} \tag{72}$$

Last but not least, we concentrate on the second term of the inequality (70)

$$\left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} p_2^{\varphi^t} \left(V_N(x_1 - x_2) - \left(V_N * |\varphi^t|^2 \right) (x_1) \right) q_1^{\varphi^t} q_2^{\varphi^t} \left| \Psi_N^t \right\rangle \right\rangle \right| \tag{73}$$

Note, the part with the convolution depends only on the variable x_1 . Since we are allowed to interchange functions based on different variables, it is possible to switch the order in the convolution term. Consequently $p_2^{\varphi^t}$ acts on $q_2^{\varphi^t}$ which gives 0, because these two projectors are orthogonal to each other. It remains

$$\left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} p_2^{\varphi^t} V_N(x_1 - x_2) q_1^{\varphi^t} q_2^{\varphi^t} \left| \Psi_N^t \right\rangle \right\rangle \right|. \tag{74}$$

Now, the problem is that both $q_i^{\varphi^t}$, $i \in \{1, 2\}$, act on the same Ψ_N^t which gives just a $\sqrt{\omega^{\varphi^t}}$. Nonetheless, this condition is not sufficient for the assumptions of the Grönwall Lemma. That is the reason why we have to interchange one $q_i^{\varphi^t}$ with the interaction term. However, in general they do not commute since V_N and $q_i^{\varphi^t}$ depend on the same variables. First, we apply Cauchy-Schwarz-inequality to separate the two $q_i^{\varphi^t}$ which leads on the one hand to $\sqrt{\omega^{\varphi^t}}$ and on the other hand to a scalar product under the square root. Now, we use the symmetry of Ψ_N^t which ensures that

$\langle\langle \Psi_N^t | q_2^{\varphi^t} | \Psi_N^t \rangle\rangle = \frac{1}{N-1} \sum_{n=2}^N \langle\langle \Psi_N^t | q_2^{\varphi^t} | \Psi_N^t \rangle\rangle$ holds true. Therefore, the diagonal terms of the scalar product are of order $\frac{1}{N}$ and the remaining terms are of order 1. However, they produce another ω^{φ^t} , since these $q_i^{\varphi^t}$ and V_N commute, because they depend on different variables. Finally, we arrive at a term which is affine with respect to ω^{φ^t} and at an error of order $\frac{1}{N}$.

$$\begin{aligned}
& \left| \langle\langle \Psi_N^t | p_1^{\varphi^t} p_2^{\varphi^t} V_N(x_1 - x_2) q_1^{\varphi^t} q_2^{\varphi^t} | \Psi_N^t \rangle\rangle \right| \\
&= \frac{1}{N-1} \left| \langle\langle \Psi_N^t | \sum_{k=2}^N p_1^{\varphi^t} p_k^{\varphi^t} V_N(x_1 - x_k) q_1^{\varphi^t} q_k^{\varphi^t} | \Psi_N^t \rangle\rangle \right| \\
&\leq \frac{1}{N-1} \left\| q_1^{\varphi^t} \Psi_N^t \right\|_2 \left\| \sum_{k=2}^N q_k^{\varphi^t} V_N(x_1 - x_k) p_1^{\varphi^t} p_k^{\varphi^t} \Psi_N^t \right\|_2 \\
&= \left\{ \frac{1}{(N-1)^2} \left(\sum_{k=2}^N \left\| q_k^{\varphi^t} V_N(x_1 - x_k) p_1^{\varphi^t} p_k^{\varphi^t} \Psi_N^t \right\|_2^2 \right. \right. \\
&\quad \left. \left. + \sum_{(k \neq l)=2}^N \left\| V_N(x_1 - x_k) p_1^{\varphi^t} p_k^{\varphi^t} q_l^{\varphi^t} \Psi_N^t \right\|_2 \left\| V_N(x_1 - x_l) p_1^{\varphi^t} p_l^{\varphi^t} q_k^{\varphi^t} \Psi_N^t \right\|_2 \right) \omega^{\varphi^t} \right\}^{\frac{1}{2}} \\
&\stackrel{(91)}{\leq} \|\varphi^t\|_{2s} \|V_N\|_{2r} \sqrt{\frac{2}{N} + \omega^{\varphi^t} \sqrt{\omega^{\varphi^t}}} \\
&\leq \|\varphi^t\|_{2s} \|V_N\|_{2r} \left(\omega^{\varphi^t} + \frac{1}{N} \right) \tag{75}
\end{aligned}$$

where we used $\sqrt{ab} \leq \frac{a+b}{2}$, $\forall a, b \geq 0$ in the last step.

To sum up, we get for the time derivative of ω^{φ^t} an upper bound.

$$\begin{aligned}
\left| \dot{\omega}^{\varphi^t} \right| &\leq 2(N-1) \left\{ 0 + \|\varphi^t\|_{2s} \|V_N\|_{2r} \left(\omega^{\varphi^t} + \frac{1}{N} \right) + 2 \|\varphi^t\|_{2s} \|V_N\|_{2r} \omega^{\varphi^t} \right\} \\
&= (N-1) \|\varphi^t\|_{2s} \|V_N\|_{2r} \left\{ 6\omega^{\varphi^t} + \frac{2}{N} \right\} \tag{76}
\end{aligned}$$

In a previous discussion, we fixed the interaction potential V_N to be scaled with $\frac{1}{N}$, compare (44). Hence, this yields to

$$\begin{aligned}
\left| \dot{\omega}^{\varphi^t} \right| &\leq (N-1) \|\varphi^t\|_{2s} \|V_N\|_{2r} \left\{ 6\omega^{\varphi^t} + \frac{2}{N} \right\} \\
&\leq \|\varphi^t\|_{2s} \|v\|_{2r} \left\{ 6\omega^{\varphi^t} + \frac{2}{N} \right\} \\
&= 6C^{\varphi^t} \omega^{\varphi^t} + \frac{2C^{\varphi^t}}{N} \tag{77}
\end{aligned}$$

with $C^{\varphi^t} = \|\varphi^t\|_{2s} \|v\|_{2r} > 0$.

3.4.4 Interpretation of the summands of the estimate

Let us have a closer look at the machinery which we introduced in this section. First of all, there is the counting operator ω^{φ^t} which determines the number of bad particles. We take for granted that in the initial state, the amount of particles which is not in the given state is small compared to the

whole number of particles. This feature is in our understanding equivalent to the claim that the N-particle state is almost a product state. Moreover, the dynamics of the whole system is known due to the N-particle Schrödinger equation.

In the following, we give a further reason, why the Hartree equation has this form, described in equation (54).

Let us start with a general interaction term $W \in L^{2r}(\mathbb{R}^3)$, moreover, we add kinetic and potential energy. Therefore we go on with this equality

$$i\partial_t \varphi^t = (-\Delta_x + A^t(x) + (N-1)W(x)) \varphi^t \quad (78)$$

We assume W to be of order $\frac{1}{N}$ such that the energy is of order 1 with respect to the particle number. According to the method, we use the time derivative of the counting measure and the Grönwall Lemma to estimate the counting measure itself from above for various times t . In the treated version, the derivative looks like

$$\begin{aligned} |\dot{\omega}^{\varphi^t}| \leq & 2(N-1) \left(\left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} p_2^{\varphi^t} (V_N(x_1 - x_2) - W(x_1)) q_1^{\varphi^t} p_2^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right| \right. \\ & + \left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} p_2^{\varphi^t} (V_N(x_1 - x_2) - W(x_1)) q_1^{\varphi^t} q_2^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right| \\ & \left. + \left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} q_2^{\varphi^t} (V_N(x_1 - x_2) - W(x_1)) q_1^{\varphi^t} q_2^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right| \right). \quad (79) \end{aligned}$$

The reason for this configuration is the dynamic of the N-particle state Ψ_N^t and the time evolution of a single boson. With other words, physics determines exactly this estimate. Now, there are two possibilities either we can show that there exists at least one $W \in L^{2r}(\mathbb{R}^3)$ for which (79) converges or the expression always diverges in the mean field limit $N \rightarrow \infty$. Our goal is to prove that the first happens. Since we apply the Grönwall Lemma at the end, and in order to succeed, we have to assure that the prefactor of ω^{φ^t} is at the most of order 1 with respect to the particle numbers. Moreover, also the additional term has to vanish in the mean field limit, such that $\omega^{\varphi^t} \xrightarrow{N \rightarrow \infty} 0$ if and only if $\omega^{\varphi^0} \xrightarrow{N \rightarrow \infty} 0$. This is a consequence of (42) under the condition that (32) holds true.

For this reason, we have a clear look at all three summands of (79). To start with the second one. In our estimate in (75), we demonstrated that

$$\left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} p_2^{\varphi^t} (V_N(x_1 - x_2) - W(x_1)) q_1^{\varphi^t} q_2^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right| \leq \|\varphi^t\|_{2s} \|V_N\|_{2r} \left(\omega^{\varphi^t} + \frac{1}{N} \right) \quad (80)$$

holds. Note, the assessment is independent of W . Besides, the additional factor $(N-1)$ from (79) and the rescaling of V_N lead to a prefactor of order 1 with respect to the particle number, as well as $\frac{1}{N}$ converges to 0 in the mean field limit. Consequently this estimate contributes to the convergence of ω^{φ^t} to 0 in the mean field limit if the initial ω^{φ^0} does.

In addition, the third term has the upper bound:

$$\left| \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} q_2^{\varphi^t} (V_N(x_1 - x_2) - W(x_1)) q_1^{\varphi^t} q_2^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right| \leq \|\varphi^t\|_{2s} (\|V_N\|_{2r} + \|W\|_{2r}) \omega^{\varphi^t} \quad (81)$$

Since we presume that $W \in L^{2r}(\mathbb{R}^3)$ is of order $\frac{1}{N}$ then for sure, $(N-1)$ times the prefactor in front of ω^{φ^t} takes finite values.

To conclude, the dynamics of Ψ_N^t and φ^t as well as the supposition that $W \in L^{2r}(\mathbb{R}^3)$ holds true, are the reason, why two terms of (79) lead to the convergence of ω^{φ^t} to 0 in the mean field limit.

Because of this, the expression

$$\left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} q_2^{\varphi^t} (V_N(x_1 - x_2) - W(x_1)) q_1^{\varphi^t} q_2^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \quad (82)$$

decides whether the introduced method passes or fails. If there exists an $W(x_1)$ in such a way, that this scalar product is negligible in the mean field limit or even vanishes, then due to Grönwall's Lemma we can make reasonable statements concerning ω^{φ^t} at arbitrary times t .

As already mentioned, physics contributes only in the second and in the third summand of (79), therefore, we have to ask the question: How can we interpret (82)?

In order to repeat, physics says that the temporal change of the number of bad particles is small. We infer this from the prefactors of ω^{φ^t} in (80) and (81). The only time dependent function is the one-particle wave function φ^t itself. Since $\varphi^t \in L^{2s}(\mathbb{R}^3)$ for any $t \in [0, T]$ and T finite, holds true, also the norm $\|\varphi^t\|_{2s}$ cannot go to infinity within short time intervals $0 < \Delta t \ll 1$. Nevertheless, the scalar product (82) declares if ω^{φ^t} counts the bad particles in the right way.

As a small remark, let us repeat, for the experiment, we prepare a huge number of bosons, each in the initial state φ^t . Because of the Brownian motion and other side effects, it is not possible to produce clean N -particle states in which every single boson is in the same state. Consequently, there is always a small amount of particles which lives in the space $\text{span}\{\varphi^t\}^\perp$. These are the *bad particles* which we want to determine with the counting measure ω^{φ^t} .

At the beginning of our experiment, at time $t = 0$, we assume for the initial state Ψ_N^0 that $\omega^{\varphi^0} \approx 0$ in the mean field limit. Then, after some short time $0 < t \ll 1$ it could be that ω^{φ^t} increases, i.e. $\omega^{\varphi^t} \approx 1$ and therefore, also the time derivative would increase drastically. Compared to (80) and (81) this means that $\|\varphi^t\|_{2s}$ would converge to infinity for $0 < t \ll 1$, but this would contradict to $\varphi^t \in L^{2s}(\mathbb{R}^3)$ for all $t \in [0, T]$. As a consequence, physics demands that $\dot{\omega}^{\varphi^t}$ is small and therefore ω^{φ^t} remains small. Because of this, (82) would go wrong if it blows up to infinity. The reason for this disturbed behavior can be interpreted as follows. In spite of counting the bad particles, the counting measure ω^{φ^t} would also declare good particles, i.e. bosons which are in the state φ^t , as bad particles.

In consequence, we have to look for an $W(x_1)$ such that (82) is negligible or even zero. However, this condition is equivalent to the statement, that we have to find a one-particle state $\phi^t \in L^{2s}(\mathbb{R}^3)$ which ensures that ω^{φ^t} counts the *bad particles* which we declared as bad particles, i.e. all bosons which are not in the state φ^t . Therefore, we have to compute

$$\begin{aligned} p_2^{\varphi^t} (V_N(x_1 - x_2) - W(x_1)) p_2^{\varphi^t} &= p_2^{\varphi^t} V_N(x_1 - x_2) p_2^{\varphi^t} - p_2^{\varphi^t} W(x_1) p_2^{\varphi^t} \\ &= p_2^{\varphi^t} \left(V_N * |\varphi^t|^2 \right) (x_1) p_2^{\varphi^t} - p_2^{\varphi^t} W(x_1) p_2^{\varphi^t} \\ &= p_2^{\varphi^t} \left(\left(V_N * |\varphi^t|^2 \right) (x_1) - W(x_1) \right) p_2^{\varphi^t}. \end{aligned} \quad (83)$$

As a result, the ϕ^t we want is identical to φ^t which represents the good states. Moreover, the interaction term of the Hartree equation has to have the form

$$W(x_1) = \left(V_N * |\varphi^t|^2 \right) (x_1). \quad (84)$$

But this is exactly the formula we already determined in the discussion in section 3.2.

To conclude, the easiest term in the calculation in section 3.4.3 which gives zero takes full responsibility for the success of this shown method and proves at the same time the correctness of the Hartree equation (54).

Finally, the well known Schrödinger equation, as well as the Hartree equation ensure the passing of the counting method.

3.4.5 Used estimates in detail

In the following, we demonstrate the used estimates of section 3.4.3. Here, $\varphi_j^t = \varphi^t(x_j)$ denotes the wave function describing the j^{th} particle.

First of all, we show the identity, which ensures that the first summand in (70) is identical to 0.

$$\begin{aligned} p_2^{\varphi^t} V_N(x_1 - x_2) p_2^{\varphi^t} &= |\varphi(x_2)\rangle \int \varphi^*(x_2) V_N(x_1 - x_2) \varphi(x_2) dx_2 \langle \varphi(x_2)| \\ &= p_2^{\varphi^t} (V_N * |\varphi|^2)(x_1) \\ &= p_2^{\varphi^t} (V_N * |\varphi|^2)(x_1) p_2^{\varphi^t} \end{aligned} \quad (85)$$

where we only apply the projector property $p_2^{\varphi^t} = \left(p_2^{\varphi^t}\right)^2$.

In the following computations, we need several times the norm of an operator which acts on a one-particle state $\phi(x_1) \in L^2(\mathbb{R}^3)$.

$$\begin{aligned} \left\| p_1^{\varphi^t} V_N^2(x_1 - x_2) p_1^{\varphi^t} \right\|_{op} &\leq \sup_{x_2 \in \mathbb{R}^3} \left\| p_1^{\varphi^t} V_N^2(x_1 - x_2) p_1^{\varphi^t} \right\|_{op} \\ &= \sup_{x_2 \in \mathbb{R}^3} \sup_{\|\phi_1\|_2=1} \left\| p_1^{\varphi^t} V_N^2(x_1 - x_2) p_1^{\varphi^t} \phi_1 \right\|_2 \\ &= \sup_{x_2 \in \mathbb{R}^3} \sup_{\|\phi_1\|_2=1} \left\langle \phi_1 \left| p_1^{\varphi^t} V_N^2(x_1 - x_2) p_1^{\varphi^t} p_1^{\varphi^t} V_N^2(x_1 - x_2) p_1^{\varphi^t} \right| \phi_1 \right\rangle^{\frac{1}{2}} \\ &= \sup_{x_2 \in \mathbb{R}^3} \sup_{\|\phi_1\|_2=1} \left(\langle \phi_1 | \varphi_1^t \rangle \langle \varphi_1^t | V_N^2(x_1 - x_2) | \varphi_1^t \rangle \langle \varphi_1^t | \varphi_1^t \rangle \langle \varphi_1^t | V_N^2(x_1 - x_2) | \varphi_1^t \rangle \langle \varphi_1^t | \phi_1 \rangle \right)^{\frac{1}{2}} \\ &= \sup_{x_2 \in \mathbb{R}^3} \langle \varphi_1^t | V_N^2(x_1 - x_2) | \varphi_1^t \rangle \sup_{\|\phi_1\|_2=1} \left\langle \phi_1 \left| p_1^{\varphi^t} \right| \phi_1 \right\rangle^{\frac{1}{2}} \\ &\leq \sup_{x_2 \in \mathbb{R}^3} \left\| \varphi^{t^2} \right\|_s \left\| V_N^2(\cdot - x_2) \right\|_r \left\| p_1^{\varphi^t} \right\|_{op} \\ &= \left\| \varphi^t \right\|_{2s}^2 \left\| V_N \right\|_{2r}^2. \end{aligned} \quad (86)$$

We take advantage of a Hölder estimate with the condition $\frac{1}{r} + \frac{1}{s} = 1$ and the fact that the initial V_N^2 is just shifted by x_2 which does not influence the norm. Moreover, the interaction and for sure the projector are selfadjoint.

Next we have to subscribe to a slight change of the term above, but with the same structure

$$\left\| p_1^{\varphi^t} \left(V_N(x_1 - x_2) - \left(V_N * |\varphi^t|^2 \right)(x_1) \right)^2 p_1^{\varphi^t} \right\|_{op}. \quad (87)$$

The estimate works just like in (86), however, we need to cover

$$\begin{aligned}
& \sup_{x_2 \in \mathbb{R}^3} \left\langle \varphi_1^t \left| \left(V_N(x_1 - x_2) - \left(V_N * |\varphi^t|^2 \right)(x_1) \right)^2 \right| \varphi_1^t \right\rangle \\
& \leq \sup_{x_2 \in \mathbb{R}^3} \left| \langle \varphi_1^t | V_N^2(x_1 - x_2) | \varphi_1^t \rangle \right| + \sup_{x_2 \in \mathbb{R}^3} \left| \left\langle \varphi_1^t \left| \left(V_N * |\varphi^t|^2 \right)^2(x_1) \right| \varphi_1^t \right\rangle \right| \\
& \quad + 2 \sup_{x_2 \in \mathbb{R}^3} \left| \left\langle \varphi_1^t \left| V_N(x_1 - x_2) \left(V_N * |\varphi^t|^2 \right)(x_1) \right| \varphi_1^t \right\rangle \right| \\
& \leq \sup_{x_2 \in \mathbb{R}^3} \left\| \varphi^{t^2} \right\|_s \left\| V_N^2(\cdot - x_2) \right\|_r + \left\| \varphi^{t^2} \right\|_s \left\| \left(V_N * |\varphi^t|^2 \right)^2(\cdot) \right\|_r \\
& \quad + 2 \sup_{x_2 \in \mathbb{R}^3} \left\| \varphi^{t^2} \right\|_s \left\| V_N(\cdot - x_2) \left(V_N * |\varphi^t|^2 \right) \right\|_r \\
& \leq \|\varphi\|_{2s}^2 \|V_N\|_{2r}^2 + \|\varphi\|_{2s}^2 \left\| V_N * |\varphi^t|^2 \right\|_{2r}^2 + 2 \|\varphi^t\|_{2s}^2 \sup_{x_2 \in \mathbb{R}^3} \|V_N(\cdot - x_2)\|_{2r} \left\| V_N * |\varphi^t|^2 \right\|_{2r} \\
& \leq \|\varphi^t\|_{2s}^2 \|V_N\|_{2r}^2 + \|\varphi^t\|_{2s}^2 \left(\|V_N\|_{2r} \left\| |\varphi^t|^2 \right\|_1 \right)^2 + 2 \|\varphi^t\|_{2s}^2 \|V_N\|_{2r} \|V_N\|_{2r} \left\| |\varphi^t|^2 \right\|_1 \\
& = \|\varphi^t\|_{2s}^2 \|V_N\|_{2r}^2 + \|\varphi^t\|_{2s}^2 \|V_N\|_{2r}^2 \|\varphi^t\|_2^4 + 2 \|\varphi^t\|_{2s}^2 \|V_N\|_{2r}^2 \|\varphi^t\|_2^2 \\
& = 4 \|\varphi^t\|_{2s}^2 \|V_N\|_{2r}^2. \tag{88}
\end{aligned}$$

In the last steps, we profit twice by the Young inequality $\|f * g\|_r \leq \|f\|_p \cdot \|g\|_q$ where $\frac{1}{p} + \frac{1}{q} = \frac{1}{r} + 1$ holds. The second inequality sign and the L^r -norm and L^s -norm come from an Hölder estimate with the condition on r and s , $\frac{1}{r} + \frac{1}{s} = 1$. Hence, we arrive at

$$\left\| p_1^{\varphi^t} \left(V_N(x_1 - x_2) - \left(V_N * |\varphi^t|^2 \right)(x_1) \right)^2 p_1^{\varphi^t} \right\|_{op} \leq 4 \|\varphi^t\|_{2s}^2 \|V_N\|_{2r}^2 \tag{89}$$

which is needed for the assessment of the third summand in (70).

Moreover, let us consider

$$\begin{aligned}
\left\| V_N(x_1 - x_2) p_1^{\varphi^t} \Phi \right\|_2 &= \left\langle \left\langle \Phi \left| p_1^{\varphi^t} V_N^2(x_1 - x_2) p_1^{\varphi^t} \right| \Phi \right\rangle \right\rangle^{\frac{1}{2}} \\
&\leq \left\| p_1^{\varphi^t} V_N^2(x_1 - x_2) p_1^{\varphi^t} \right\|_{op}^{\frac{1}{2}} \|\Phi\|_2 \\
&\stackrel{(86)}{\leq} \|\varphi^t\|_{2s} \|V_N\|_{2r} \|\Phi\|_2 \tag{90}
\end{aligned}$$

which helps to estimate the second term of (70) on which we concentrate now.

$$\begin{aligned}
& \left\| q_2^{\varphi^t} V_N(x_1 - x_2) p_1^{\varphi^t} p_2^{\varphi^t} \Psi_N^t \right\|_2 \\
&= \left\| \frac{1}{N-1} \sum_{k=2}^N q_k^{\varphi^t} V_N(x_1 - x_k) p_1^{\varphi^t} p_k^{\varphi^t} \Psi_N^t \right\|_2 \\
&= \left\{ \frac{1}{(N-1)^2} \left(\sum_{k=2}^N \left\| q_k^{\varphi^t} V_N(x_1 - x_k) p_1^{\varphi^t} p_k^{\varphi^t} \Psi_N^t \right\|_2^2 \right. \right. \\
&\quad \left. \left. + \sum_{(k \neq l)=2}^N \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} p_k^{\varphi^t} V_N(x_1 - x_k) q_k^{\varphi^t} q_l^{\varphi^t} V_N(x_1 - x_l) p_1^{\varphi^t} p_l^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right) \right\}^{\frac{1}{2}} \\
&\leq \left\{ \frac{1}{(N-1)^2} \left(\sum_{k=2}^N \left\| q_k^{\varphi^t} \right\|_{op}^2 \left\| V_N(x_1 - x_k) p_1^{\varphi^t} p_k^{\varphi^t} \Psi_N^t \right\|_2^2 \right. \right. \\
&\quad \left. \left. + \sum_{(k \neq l)=2}^N \left\langle \left\langle \Psi_N^t \left| p_1^{\varphi^t} p_k^{\varphi^t} q_l^{\varphi^t} V_N(x_1 - x_k) V_N(x_1 - x_l) p_1^{\varphi^t} p_l^{\varphi^t} q_k^{\varphi^t} \right| \Psi_N^t \right\rangle \right\rangle \right) \right\}^{\frac{1}{2}} \\
&\leq \left\{ \frac{1}{(N-1)^2} \left(\sum_{k=2}^N \left\| V_N(x_1 - x_k) p_1^{\varphi^t} p_k^{\varphi^t} \Psi_N^t \right\|_2^2 \right. \right. \\
&\quad \left. \left. + \sum_{(k \neq l)=2}^N \left\| V_N(x_1 - x_k) p_1^{\varphi^t} p_k^{\varphi^t} q_l^{\varphi^t} \Psi_N^t \right\|_2 \left\| V_N(x_1 - x_l) p_1^{\varphi^t} p_l^{\varphi^t} q_k^{\varphi^t} \Psi_N^t \right\|_2 \right) \right\}^{\frac{1}{2}} \\
&\stackrel{(90)}{\leq} \left\{ \frac{1}{(N-1)^2} \left(\sum_{k=2}^N \|\varphi^t\|_{2s}^2 \|V_N\|_{2r}^2 \left\| p_k^{\varphi^t} \Psi_N^t \right\|_2^2 \right. \right. \\
&\quad \left. \left. + \sum_{(k \neq l)=2}^N \|\varphi^t\|_{2s}^2 \|V_N\|_{2r}^2 \left\| q_l^{\varphi^t} \Psi_N^t \right\|_2 \left\| q_k^{\varphi^t} \Psi_N^t \right\|_2 \right) \right\}^{\frac{1}{2}} \\
&= \|\varphi^t\|_{2s} \|V_N\|_{2r} \left\{ \frac{1}{(N-1)^2} \left((N-1) + ((N-1)^2 - (N-1)) \omega^{\varphi^t} \right) \right\}^{\frac{1}{2}} \\
&= \|\varphi^t\|_{2s} \|V_N\|_{2r} \left\{ \frac{1}{N-1} + \frac{N-2}{N-1} \omega^{\varphi^t} \right\}^{\frac{1}{2}} \\
&\leq \|\varphi^t\|_{2s} \|V_N\|_{2r} \sqrt{\frac{2}{N} + \omega^{\varphi^t}} \tag{91}
\end{aligned}$$

The symbol $\sum_{(k \neq l)=2}^N$ describes the sum over k and l , both from 2 to N but k and l always differ from each other.

3.4.6 The convergence behavior of the upper bound

After having estimated $|\dot{\omega}^{\varphi^t}|$, we can compare the estimate to the statement of Grönwall's Lemma. Remember, the final result of section 3.4.3 is

$$\begin{aligned}
|\dot{\omega}^{\varphi^t}| &\leq \|\varphi^t\|_{2s} \|v\|_{2r} \left\{ 6\omega^{\varphi^t} + \frac{2}{N} \right\} \\
&= 6C^{\varphi^t} \omega^{\varphi^t} + \frac{2C^{\varphi^t}}{N}. \tag{92}
\end{aligned}$$

To conclude, the time dependent number of particles ω^{φ^t} has an upper bound

$$\begin{aligned}\omega^{\varphi^t} &\leq e^{\int_0^t 6\|\varphi^\tau\|_{2s}\|v\|_{2r}d\tau} \left(\omega^{\varphi^0} + \int_0^t 2\|\varphi^{\tilde{t}}\|_{2s}\|v\|_{2r} \frac{1}{N} e^{-\int_0^{\tilde{t}} 6\|\varphi^\tau\|_{2s}\|v\|_{2r}d\tau} d\tilde{t} \right) \\ &= e^{\int_0^t 6C^{\varphi^\tau}d\tau} \left(\omega^{\varphi^0} + \frac{2}{N} \int_0^t C^{\varphi^{\tilde{t}}} e^{-\int_0^{\tilde{t}} 6C^{\varphi^\tau}d\tau} d\tilde{t} \right)\end{aligned}\quad (93)$$

which converges to 0 in the mean field limit. Now, we have to declare, under which conditions the upper inequality produces useful results. At the beginning, in section 1 was a discussion about the assumption

$$\mu^{\Psi_N^0} \xrightarrow{N \rightarrow \infty} |\varphi^0\rangle\langle\varphi^0| \quad \text{in operator norm.} \quad (94)$$

This equals in the language of counting bad particles to

$$\omega^{\varphi^0} \xrightarrow{N \rightarrow \infty} 0. \quad (95)$$

Besides, we take for granted that $v \in L^{2r}(\mathbb{R}^3)$ and $\varphi^t \in L^{2s}(\mathbb{R}^3)$, where r and s are connected via the Hölder condition $\frac{1}{r} + \frac{1}{s} = 1$. By the way, $\|v\|_{2r}$ is constant with respect to time t . However, $\|\varphi^t\|_{2s}$ is for sure smaller than infinity, for every $t \in [0, T]$, where T picks up finite or infinite values.

Therefore, we can be sure that ω^{φ^t} never runs out to infinity, since $C^{\varphi^t} = \|\varphi^t\|_{2s}\|v\|_{2r}$ is a constant with respect to the particle number N .

We deal now with $\{\omega_N^{\varphi^t}\}_{N \in \mathbb{N}}$ as a time dependent sequence in \mathbb{R}_0^+ , where we just add the concerning particle number in the notation. First of all we consider the finite case $T < \infty$. Since $\varphi^t \in L^{2s}(\mathbb{R}^3)$ holds for all $t \in [0, T]$ and t is always finite, also the time integration of the constant $C^{\varphi^t} = \|\varphi^t\|_{2s}\|v\|_{2r}$ gives a finite value. That is the reason, why ω^{φ^t} is bounded from above and cannot blow up to infinity. Furthermore, taking the mean field limit $N \rightarrow \infty$ on both sides of (93), we observe that $\omega^{\varphi^t} \xrightarrow{N \rightarrow \infty} 0$ since $\omega^{\varphi^0} \xrightarrow{N \rightarrow \infty} 0$ and the second summand vanishes with $\frac{1}{N}$. Moreover the remaining prefactors are in the expression constant with respect to the particle number and do not influence the mean field limit.

Besides, $\omega_N^{\varphi^t}$ even converges uniformly in t . In order to show this, we introduce the two time dependent, finite and positive functions

$$\Gamma^t = e^{\int_0^t 6\|\varphi^\tau\|_{2s}\|v\|_{2r}d\tau} \quad (96)$$

$$\Lambda^t = 2\|v\|_{2r} \int_0^t \|\varphi^{\tilde{t}}\|_{2s} e^{-\int_0^{\tilde{t}} 6\|\varphi^\tau\|_{2s}\|v\|_{2r}d\tau} d\tilde{t}. \quad (97)$$

Since $\omega_N^{\varphi^0}$ and $\frac{1}{N}$ converge to 0 for $N \rightarrow \infty$ there exist for all $\epsilon > 0$ an $M_\epsilon \in \mathbb{N}$ such that $\omega_N^{\varphi^0} < \frac{\epsilon}{2\Gamma_{max}}$ and $\frac{\Lambda_{max}}{N} < \frac{\epsilon}{2}$ hold true for every $N > M_\epsilon$. Here Γ_{max} is defined as the maximum of Γ^t over all $t \in [0, T]$ and $T < \infty$, analogously is the definition of Λ_{max} . Consequently

$$\left| \omega_N^{\varphi^t} - 0 \right| = \omega_N^{\varphi^t} \leq \Gamma^t \cdot \omega_N^{\varphi^0} + \frac{\Lambda^t}{N} < \epsilon \quad (98)$$

holds true for all $N > M_\epsilon$ and for all $t \in [0, T]$ with $T < \infty$. Hence $\left\{ \omega_N^{\varphi^t} \right\}_{N \in \mathbb{N}}$ converges uniformly for finite t .

Second, we increase the time interval and set T to infinity. In order to ensure furthermore that $\omega_N^{\varphi^t}$ converges to 0 as N goes to infinity for any $t \in [0, \infty)$ we have to append a new condition. That is the reason why $\int_0^\infty \|\varphi^t\|_{2s} dt < \infty$ has to hold. As a consequence of this property, the time dependent functions Λ^t and Γ^t are finite for all $t \in [0, \infty)$ and hence $\left\{ \omega_N^{\varphi^t} \right\}_{N \in \mathbb{N}}$ also converges uniformly for any $t \in \mathbb{R}_0^+$.

4 Conclusion

To sum up, if the number of bad particles converges to 0 in the mean field limit N going to infinity at time $t=0$, then the number of bad particles at any arbitrary time t has the same property. Equivalently, if the initial reduced one-particle density matrix converges in operator norm to the pure one-particle state φ^0

$$\mu^{\Psi_N^0} \xrightarrow{N \rightarrow \infty} |\varphi^0\rangle \langle \varphi^0| \quad (99)$$

then also

$$\mu^{\Psi_N^t} \xrightarrow{N \rightarrow \infty} |\varphi^t\rangle \langle \varphi^t| \quad (100)$$

is valid in operator norm for any time t . Consequently, all initial (almost) product states of a bosonic N -particle system remain (almost) product states for all times t and large particle numbers although there is interaction between the particles themselves.

Finally, to conclude, it is neither obvious nor intuitive that the number of bad particles in a bosonic N -particle system converges to 0 in the mean field limit at any time if it converges to 0 at the beginning, due to the fact that there is interaction and therefore correlation between the particles.

Part III

Time Evolution of a Bosonic System with Two Different Types

Up to this moment, we considered the time evolution of a bosonic many particle system, e.g. a Bose-Einstein-Condensate, with one type of particles. In the following, we treat two different kinds of bosons mixed up in one system. Moreover, as in the issue which we already considered, there occurs pair interaction between all particles. The goal is to determine the time evolution of the number of bad particles in the whole system. Beyond, we take for granted that the number of bad particles in the initial state vanishes in the mean field limit $N \rightarrow \infty$ and $M \rightarrow \infty$, or vice versa. This corresponds to the analysis of the temporal behavior of the reduced one-particle density matrix. With other words, we would like to know if (almost) product states remain (almost) product states for all finite or infinite times t . For the sake of simplicity, we study the physical behavior under the assumption that we only allow pair interaction. While interaction of higher order would not change the general statement of the result. In contrast to the second part, we have now two distinguishable types of bosons and hence, there is interaction between the bosons of one species as well as the interaction between the different types.

5 Notation, Definitions and General Discussion

5.1 The Hamiltonian and the general wave function

Let us start with a few comments on the notation and a few definitions. We deal with two different bosonic particle characters, call them A and B. The number of particles of type A is N , whereas the number of particles of type B is M . Besides we label the particles of the species A with x_1, \dots, x_N ; while we prescribe the bosons of type B with x_{N+1}, \dots, x_{N+M} . These particles move with a kinetic energy in perhaps two different, time dependent, potentials A^t and B^t . There is the interaction between bosons of the same sort as well as between different types. In order to be as general as possible, we assume to treat different kinds of interactions, labeled with V_A, V_B and V_{AB} which only depend on the distance of the two involved particles.

To conclude, the Hamiltonian of the whole system H_{AB} looks like

$$\begin{aligned}
 H_{AB} &= \sum_{n=1}^N (-\Delta_n) + \sum_{n=1}^N A^t(x_n) + \sum_{1 \leq j < k \leq N} V_A(x_j - x_k) \\
 &+ \sum_{m=N+1}^{N+M} (-\Delta_m) + \sum_{m=N+1}^{N+M} A^t(x_m) + \sum_{N+1 \leq j < k \leq N+M} V_B(x_j - x_k) \\
 &+ \sum_{n=1}^N \sum_{m=N+1}^{N+M} V_{AB}(x_n - x_m) \\
 &= H_A + H_B + \sum_{n=1}^N \sum_{m=N+1}^{N+M} V_{AB}(x_n - x_m).
 \end{aligned} \tag{101}$$

The Hamiltonians H_A and H_B are defined as in (43). As before, we have to discuss the order of the interactions concerning the particle numbers which ensure that we work with a balanced system. Where balanced is in the sense of neither the kinetic plus potential term nor the interaction dominates the total energy. We choose to rescale each interaction with the number of particles which is affected, i.e.

$$V_A(x) = \frac{1}{N} v_A(x) \quad (102a)$$

$$V_B(y) = \frac{1}{M} v_B(y) \quad (102b)$$

$$V_{AB}(z) = \frac{1}{N+M} v_{AB}(z). \quad (102c)$$

Because of this determination we recognize that the first line of (101) is of order N , the second of order M and the third line is of order $\frac{N \cdot M}{N+M}$. If we presume that we deal with particle numbers of the same quantity, i.e. $N \approx M$, then there is a balanced contribution of all terms in (101) to the energy of the whole system. However, if we take for granted that one type of particles dominates the whole number then, how it is expected, we can assume, that the system consists only of this one type of bosons, while we neglect the other type in question of energy.

To continue, the $N+M$ -particle state, called Ψ_{AB}^t , is defined on $L^2(\mathbb{R}^{3N} \times \mathbb{R}^{3M})$, moreover, we choose it normalized. Furthermore, the function

$$\Psi_{AB}^t = \Psi_{AB}^t(x_1, \dots, x_N, x_{N+1}, \dots, x_{N+M}) \quad (103)$$

has to be symmetric under particle exchange, on the one hand in the first N variables x_1, \dots, x_N which represent the particle type A, and on the other hand in the variables x_{N+1}, \dots, x_{N+M} standing for the particles of type B. The reason for that behavior is the bosonic character of the treated particles. Note, we stress that there is no exchange in-between the different types.

In this circumstance a product state has the form

$$\Psi_{AB}^t = \prod_{j=1}^N \varphi_A^t(x_j) \prod_{k=N+1}^{N+M} \varphi_B^t(x_k). \quad (104)$$

Therefore, the calculation of the reduced one-particle density matrix yields to

$$\mu^{\Psi_{AB}^t}(x_j) = \delta_{j \in \{1, \dots, N\}} |\varphi_A^t(x_j)\rangle \langle \varphi_A^t(x_j)| + \delta_{j \in \{N+1, \dots, N+M\}} |\varphi_B^t(x_j)\rangle \langle \varphi_B^t(x_j)| \quad (105)$$

where $\delta_{j \in \{1, \dots, N\}}$ is the δ -function which gives 1 if $j \in \{1, \dots, N\}$ and 0 otherwise. In general, this notation expresses the fact that we integrate over all $N+M$ particles but not over the particle x_j .

Moreover, an almost product state Ψ_{AB}^t in this case reads without the normalization constant as

$$\Psi_{AB}^t = \left(\chi_A^t(x_1, \dots, x_N) \cdot \prod_{j=1}^N \varphi_A^t(x_j) \right)_{sym.} \cdot \left(\chi_B^t(x_{N+1}, \dots, x_{N+M}) \cdot \prod_{j=N+1}^{N+M} \varphi_B^t(x_j) \right)_{sym.} \quad (106)$$

where χ_A contains all n bad particles of type A and is perpendicular in the way we already discussed in section 1.2. The same holds for the bosons of species B. Therefore, we can split up the $N+M$ -particle state into the product of two normalized wave functions consisting of only one type, hence

$$\Psi_{AB}^t(x_1, \dots, x_{N+M}) = \psi_A^t(x_1, \dots, x_N) \cdot \psi_B^t(x_{N+1}, \dots, x_{N+M}) \quad (107)$$

with $\psi_A \in L^2(\mathbb{R}^{3N})$ and $\psi_B \in L^2(\mathbb{R}^{3M})$ as well as $\|\psi_A\|_2 = 1 = \|\psi_B\|_2$ holds true.

5.2 The Hartree equations of the two different species

Let us have a closer look at the Hartree equations of the normalized one-particle states φ_A^t and φ_B^t , respectively.

$$i\partial_t\varphi_A^t = \left(-\Delta + A^t + (N-1)\left(V_A * |\varphi_A^t|^2\right) + M\left(V_{AB} * |\varphi_B^t|^2\right)\right)\varphi_A^t \quad (108)$$

$$i\partial_t\varphi_B^t = \left(-\Delta + B^t + (M-1)\left(V_B * |\varphi_B^t|^2\right) + N\left(V_{AB} * |\varphi_A^t|^2\right)\right)\varphi_B^t \quad (109)$$

We concentrate now only on equation (108) because the other equality reflects the same properties. As in section 3.2, the particles of type A move in a potential and interact with the remaining N-1 particles of the same species. However, these bosons are also allowed to interact with all M particles of type B expressing the last term in (108). We infer the equality, especially the interaction term of the Hartree equations of (108) and (109) from the previous discussion in section 3.2 and 3.4.4. Remember that $|\varphi_A^t|^2$ and $|\varphi_B^t|^2$ respectively are, like before empirical densities, connected to a large number of particles of both types A and B.

Moreover, let us consider the orders with respect to the particle numbers of the interactions between the different species A and B. By the way, the remaining terms in (108) and (109) should all be of order one since the kinetic energy as well as the potential is of this order. For the last terms, we receive order $\frac{M}{N+M}$ in (108) and we arrive at $\frac{N}{N+M}$ in (109). Therefore, in the case $N \approx M$ every term in (108) and (109) is of order one. However, if we assume $N \gg M$, then the interaction of an A-particle with an B-particle can be neglected, because as a boson of type A, most of the particles around are of the same type. Whereas, a particle of species B interacts with a huge number of A-particles, for the same reason. As a consequence, we have to take care of this term in (109).

To conclude, this consideration agrees with the intuitive comprehension of interaction concerning systems of different types and particle numbers. Because of that, the choice of the rescaling of the potentials in (102) is one reasonable solution.

6 Time Evolution of the Ratio of Bad Particles

In the following, we want to study the time evolution of the number of bad particles in view of the fact that the system which we treat, consists of two different types of bosons where pair interaction takes place between all bosons.

6.1 The counting operator

We follow the strategy which we presented in the second part. For that reason, we again estimate from above the time derivative of the ratio of bad particles which we call now Ω , in order to apply then Grönwall's Lemma. Let us continue with the counting operator which determines the ratio of bad bosons. By the way, as before, we do only care about the amount of bad particles therefore, we do not distinguish between different species. As a consequence, each bad boson is one of the N+M particles and for that reason is weighted with $\frac{1}{N+M}$.

In order to ascertain the ratio of bad particles, we take advantage of an counting operator running through all possible combinations of bad particles of type A and B. Consequently, we have to compute $\frac{n+m}{N+M} P_n^{\varphi_A^t} P_m^{\varphi_B^t}$ summed up over the bad particles n and m. Besides $P_m^{\varphi_B^t}$ is defined as

$$P_m^{\varphi_B^t} = \left(\prod_{j=N+1}^{N+m} q_j^{\varphi_B^t} \prod_{j=N+m+1}^{N+M} p_j^{\varphi_B^t} \right)_{sym.} \quad (110)$$

Finally, the ratio of bad particles in an N+M-particle state is labeled with Ω and defined as

$$\begin{aligned}
\Omega(t) &= \left\langle \left\langle \Psi_{AB}^t \left| \sum_{n=0}^N \sum_{m=0}^M \frac{n+m}{N+M} P_n^{\varphi_A^t} P_m^{\varphi_B^t} \right| \Psi_{AB}^t \right\rangle \right\rangle \\
&= \left\langle \left\langle \Psi_{AB}^t \left| \sum_{n=0}^N \frac{n}{N+M} P_n^{\varphi_A^t} \sum_{m=0}^M P_m^{\varphi_B^t} \right| \Psi_{AB}^t \right\rangle \right\rangle \\
&\quad + \left\langle \left\langle \Psi_{AB}^t \left| \sum_{m=0}^M \frac{m}{N+M} P_m^{\varphi_B^t} \sum_{n=0}^N P_n^{\varphi_A^t} \right| \Psi_{AB}^t \right\rangle \right\rangle \\
&= \left\langle \left\langle \Psi_{AB}^t \left| \sum_{n=0}^N \frac{n}{N+M} P_n^{\varphi_A^t} \right| \Psi_{AB}^t \right\rangle \right\rangle + \left\langle \left\langle \Psi_{AB}^t \left| \sum_{m=0}^M \frac{m}{N+M} P_m^{\varphi_B^t} \right| \Psi_{AB}^t \right\rangle \right\rangle \\
&= \Omega_A(t) + \Omega_B(t).
\end{aligned} \tag{111}$$

It is allowed to interchange and reshuffle the sums, even if $N, M \rightarrow \infty$ since all summands are nonnegative and the sums are always finite. The sum $\sum_{n=0}^N P_n^{\varphi_A^t}$ is equal to the identity because every N+M particle state has between 0 and N bad particles of type A. A mathematical proof is given in equation (22).

For these reasons, the equation (111) holds true and we can continue the computation of $\Omega(t)$ by profiting by the strategy presented in section 3.

6.2 Preparing estimates for Grönwall's Lemma

In the following, we first concentrate on the estimate of $\Omega_A(t)$ concerning the type A, afterwards, we infer from this result the expression $\Omega_B(t)$ by interchanging A with B and N with M, respectively.

With the help of equation (24) we simplify $\Omega_A(t)$ to

$$\Omega_A(t) = \left\langle \left\langle \Psi_{AB}^t \left| \sum_{n=0}^N \frac{n}{N+M} P_n^{\varphi_A^t} \right| \Psi_{AB}^t \right\rangle \right\rangle = \frac{N}{N+M} \left\langle \left\langle \Psi_{AB}^t \left| q_l^{\varphi_A^t} \right| \Psi_{AB}^t \right\rangle \right\rangle = \frac{N}{N+M} \omega^{\varphi_A^t} \tag{112}$$

where $l \in \{1, \dots, N\}$ is arbitrary since we deal with a system of bosons. As seen above, it is possible to connect $\Omega_A(t)$ with $\omega^{\varphi_A^t}$. The latter just refers to the ratio of bad particles of type A, i.e. every particle is weighted with $\frac{1}{N}$, whereas $\Omega_A(t)$ includes all N+M particles. The integration over the variables x_{N+1}, \dots, x_{N+M} simplifies to 1 for reasons of normalization. In order to use Grönwall's Lemma, we take the derivative of this expression with respect to time t. Besides, this is similar to equality (46), therefore we get

$$\dot{\Omega}_A(t) = i \frac{N}{N+M} \left\langle \left\langle \Psi_{AB}^t \left[\left[H_{AB} - h_A(x_1), q_1^{\varphi_A^t} \right] \right] \Psi_{AB}^t \right\rangle \right\rangle. \tag{113}$$

Here, H_{AB} is the Hamiltonian of the whole system and $h_A(x_1)$ is the Hamiltonian for the particle x_1 . Notice, operators which act on different particles commute, therefore we simplify the commutator above to

$$\begin{aligned}
& \left[H_{AB} - h_A(x_1), q_1^{\varphi_A^t} \right] \\
&= \left[\sum_{k=2}^N V_A(x_1 - x_k) + \sum_{m=N+1}^{N+M} V_{AB}(x_1 - x_m) - (N-1) \left(V_A * |\varphi_A^t|^2 \right) (x_1) \right. \\
&\quad \left. - M \left(V_{AB} * |\varphi_B^t|^2 \right) (x_1), q_1^{\varphi_A^t} \right] \\
&= \left[(N-1)V_A(x_1 - x_2) + M \cdot V_{AB}(x_1 - x_{N+1}) - (N-1) \left(V_A * |\varphi_A^t|^2 \right) (x_1) \right. \\
&\quad \left. - M \left(V_{AB} * |\varphi_B^t|^2 \right) (x_1), q_1^{\varphi_A^t} \right] \\
&= (N-1) \left[V_A(x_1 - x_2) - \left(V_A * |\varphi_A^t|^2 \right) (x_1), q_1^{\varphi_A^t} \right] \\
&\quad + M \left[V_{AB}(x_1 - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right) (x_1), q_1^{\varphi_A^t} \right] \tag{114}
\end{aligned}$$

where we used again that we treat a bosonic system and for that reason we can combine each sum of pair interactions in one pair interaction multiplied by the number of summands. As a consequence, we receive

$$\begin{aligned}
\dot{\Omega}_A(t) &= i \frac{N}{N+M} (N-1) \left\langle \left\langle \Psi_{AB}^t \left[V_A(x_1 - x_2) - \left(V_A * |\varphi_A^t|^2 \right) (x_1), q_1^{\varphi_A^t} \right] \middle| \Psi_{AB}^t \right\rangle \right\rangle \\
&\quad + i \frac{N}{N+M} \cdot M \cdot \left\langle \left\langle \Psi_{AB}^t \left[V_{AB}(x_1 - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right) (x_1), q_1^{\varphi_A^t} \right] \middle| \Psi_{AB}^t \right\rangle \right\rangle. \tag{115}
\end{aligned}$$

The first term above is up to the prefactor identical to expression (66). The dependence concerning particle type B integrates out, because of the normalization of ψ_B^t . Consequently, we only have to care about the second term. However, also in this case we follow the introduced strategy. Therefore we summarize the difference of the two interactions in the second expression to $f(x_1, x_{N+1})$. Moreover, since we do not know, how these interactions act on the N+M-particle state, we again introduce a few identities

$$\begin{aligned}
& \left\langle \left\langle \Psi_{AB}^t \left[V_{AB}(x_1 - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right) (x_1), q_1^{\varphi_A^t} \right] \middle| \Psi_{AB}^t \right\rangle \right\rangle \\
&= \left\langle \left\langle \Psi_{AB}^t \middle| f(x_1, x_{N+1}) q_1^{\varphi_A^t} \middle| \Psi_{AB}^t \right\rangle \right\rangle - \left\langle \left\langle \Psi_{AB}^t \middle| q_1^{\varphi_A^t} f(x_1, x_{N+1}) \middle| \Psi_{AB}^t \right\rangle \right\rangle \\
&= \left\langle \left\langle \Psi_{AB}^t \middle| \left(p_1^{\varphi_A^t} + q_1^{\varphi_A^t} \right) \left(p_{N+1}^{\varphi_B^t} + q_{N+1}^{\varphi_B^t} \right) f(x_1, x_{N+1}) q_1^{\varphi_A^t} \left(p_{N+1}^{\varphi_B^t} + q_{N+1}^{\varphi_B^t} \right) \middle| \Psi_{AB}^t \right\rangle \right\rangle \\
&\quad - \left\langle \left\langle \Psi_{AB}^t \middle| q_1^{\varphi_A^t} \left(p_{N+1}^{\varphi_B^t} + q_{N+1}^{\varphi_B^t} \right) f(x_1, x_{N+1}) \left(p_1^{\varphi_A^t} + q_1^{\varphi_A^t} \right) \left(p_{N+1}^{\varphi_B^t} + q_{N+1}^{\varphi_B^t} \right) \middle| \Psi_{AB}^t \right\rangle \right\rangle. \tag{116}
\end{aligned}$$

The only terms which survive for the same reason as in section 3.4.3 are

$$\begin{aligned}
\text{A)} & p_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} f(x_1, x_{N+1}) q_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} - q_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} f(x_1, x_{N+1}) p_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} \\
\text{B)} & p_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} f(x_1, x_{N+1}) q_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} - q_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} f(x_1, x_{N+1}) p_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} \\
\text{C)} & p_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} f(x_1, x_{N+1}) q_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} - q_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} f(x_1, x_{N+1}) p_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t}
\end{aligned}$$

Note, each term appears with its complex conjugate and since we are only interested in the absolute value of $\Omega_A(t)$, it is enough to study only the first expression of each line.

Nevertheless, in order to keep this section clear and to avoid confusion due to too much calculations, we add the computations in detail in section 6.4 like before. We only want to attach

importance to the idea of the estimate. As in part II, the numbers r and s are linked via the Hölder condition $\frac{1}{r} + \frac{1}{s} = 1$.

To start with A)

$$\left| \left\langle \left\langle \Psi_{AB}^t \left| p_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} \left(V_{AB}(x_1 - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right)(x_1) \right) q_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} \left| \Psi_{AB}^t \right\rangle \right\rangle \right| = 0 \quad (117)$$

since we know that the identity $p_{N+1}^{\varphi_B^t} V_{AB}(x_1 - x_{N+1}) p_{N+1}^{\varphi_B^t} = p_{N+1}^{\varphi_B^t} \left(V_{AB} * |\varphi_B^t|^2 \right)(x_1) p_{N+1}^{\varphi_B^t}$ holds which was already shown in (85).

As in section 3.4.3 we continue with term C)

$$\begin{aligned} & \left| \left\langle \left\langle \Psi_{AB}^t \left| p_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \left(V_{AB}(x_1 - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right)(x_1) \right) q_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \left| \Psi_{AB}^t \right\rangle \right\rangle \right| \\ & \leq \left\| q_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2 \left\| \left(V_{AB}(x_1 - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right)(x_1) \right) p_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2 \\ & \leq \|\varphi_A^t\|_{2s} \|V_{AB}\|_{2r} \left(\omega^{\varphi_A^t} + \omega^{\varphi_B^t} \right). \end{aligned} \quad (118)$$

Last but not least, we concentrate on term B)

$$\begin{aligned} & \left| \left\langle \left\langle \Psi_{AB}^t \left| p_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} \left(V_{AB}(x_1 - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right)(x_1) \right) q_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \left| \Psi_{AB}^t \right\rangle \right\rangle \right| \\ & = \left| \left\langle \left\langle \Psi_{AB}^t \left| p_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} V_{AB}(x_1 - x_{N+1}) q_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \left| \Psi_{AB}^t \right\rangle \right\rangle \right| \\ & \leq \left\| q_1^{\varphi_A^t} V_{AB}(x_1 - x_{N+1}) p_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2 \left\| q_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2 \\ & = \left\| \frac{1}{N} \sum_{k=1}^N q_k^{\varphi_A^t} V_{AB}(x_k - x_{N+1}) p_k^{\varphi_A^t} p_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2 \sqrt{\omega^{\varphi_B^t}} \\ & \stackrel{(128)}{\leq} \|\varphi_A^t\|_{2s} \|V_{AB}\|_{2r} \sqrt{\left(\frac{1}{N} + \omega^{\varphi_A^t} \right) \omega^{\varphi_B^t}} \\ & \leq \frac{1}{2} \|\varphi_A^t\|_{2s} \|V_{AB}\|_{2r} \left(\omega^{\varphi_A^t} + \omega^{\varphi_B^t} + \frac{1}{N} \right). \end{aligned} \quad (119)$$

Again, in the second part $p_{N+1}^{\varphi_B^t}$ commutes with the interaction term of the mean field Hamiltonian and acts directly on $q_{N+1}^{\varphi_B^t}$ which gives 0. At the end we use $\sqrt{ab} \leq \frac{a+b}{2} \forall a, b \in \mathbb{R}^+$.

To sum up, we arrive at

$$\begin{aligned} |\dot{\Omega}_A(t)| &= \frac{N}{N+M} (N-1) \left\langle \left\langle \Psi_{AB}^t \left| \left[V_A(x_1 - x_2) - \left(V_A * |\varphi_A^t|^2 \right)(x_1), q_1^{\varphi_A^t} \right] \left| \Psi_{AB}^t \right\rangle \right\rangle \right. \\ & \quad \left. + \frac{N}{N+M} \cdot M \cdot \left\langle \left\langle \Psi_{AB}^t \left| \left[V_{AB}(x_1 - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right)(x_1), q_1^{\varphi_A^t} \right] \left| \Psi_{AB}^t \right\rangle \right\rangle \right. \right. \\ & \leq \frac{N(N-1)}{N+M} \|\varphi_A^t\|_{2s} \|V_A\|_{2r} \left(6\omega^{\varphi_A^t} + \frac{2}{N} \right) \\ & \quad + 2 \frac{N \cdot M}{N+M} \left(0 + \frac{1}{2} \|\varphi_A^t\|_{2s} \|V_{AB}\|_{2r} \left(\omega^{\varphi_A^t} + \omega^{\varphi_B^t} + \frac{1}{N} \right) + \|\varphi_A^t\|_{2s} \|V_{AB}\|_{2r} \left(\omega^{\varphi_A^t} + \omega^{\varphi_B^t} \right) \right) \\ & \leq \frac{N^2}{N+M} \|\varphi_A^t\|_{2s} \|V_A\|_{2r} \left(6\omega^{\varphi_A^t} + \frac{2}{N} \right) \\ & \quad + \frac{N \cdot M}{N+M} \|\varphi_A^t\|_{2s} \|V_{AB}\|_{2r} \left(3\omega^{\varphi_A^t} + 3\omega^{\varphi_B^t} + \frac{1}{N} \right). \end{aligned} \quad (120)$$

Since $\Omega_A(t)$ and $\Omega_B(t)$ are absolutely identical in the structure, we get the same result for $|\dot{\Omega}_B(t)|$ by interchanging the types A and B and the particle numbers N and M. To conclude, the absolute value of the time derivative of the number of bad particles compared to the whole number of particles $|\dot{\Omega}(t)|$ can be bounded from above

$$\begin{aligned} |\dot{\Omega}(t)| &\leq \frac{N^2}{N+M} \|\varphi_A^t\|_{2s} \|V_A\|_{2r} \left(6\omega^{\varphi_A^t} + \frac{2}{N}\right) \\ &\quad + \frac{M^2}{N+M} \|\varphi_B^t\|_{2s} \|V_B\|_{2r} \left(6\omega^{\varphi_B^t} + \frac{2}{M}\right) \\ &\quad + \frac{N \cdot M}{N+M} \|\varphi_A^t\|_{2s} \|V_{AB}\|_{2r} \left(3\omega^{\varphi_A^t} + 3\omega^{\varphi_B^t} + \frac{1}{N}\right) \\ &\quad + \frac{N \cdot M}{N+M} \|\varphi_B^t\|_{2s} \|V_{AB}\|_{2r} \left(3\omega^{\varphi_B^t} + 3\omega^{\varphi_A^t} + \frac{1}{M}\right). \end{aligned} \quad (121)$$

However, that is not the end of the story, in order to use Grönwall's Lemma, we have to estimate the derivative of a function with the function itself. For that reason, we have to use some more algebra and we insert the identities (102a), (102b) and (102c) which show explicitly the dependency to the particle number of each interaction. It follows

$$\begin{aligned} |\dot{\Omega}(t)| &\leq \frac{N}{N+M} \|\varphi_A^t\|_{2s} \|v_A\|_{2r} \left(6\omega^{\varphi_A^t} + \frac{2}{N}\right) \\ &\quad + \frac{M}{N+M} \|\varphi_B^t\|_{2s} \|v_B\|_{2r} \left(6\omega^{\varphi_B^t} + \frac{2}{M}\right) \\ &\quad + \frac{N \cdot M}{(N+M)^2} \|\varphi_A^t\|_{2s} \|v_{AB}\|_{2r} \left(3\omega^{\varphi_A^t} + 3\omega^{\varphi_B^t} + \frac{1}{N}\right) \\ &\quad + \frac{N \cdot M}{(N+M)^2} \|\varphi_B^t\|_{2s} \|v_{AB}\|_{2r} \left(3\omega^{\varphi_B^t} + 3\omega^{\varphi_A^t} + \frac{1}{M}\right). \end{aligned} \quad (122)$$

For simplicity, we define

$$\|\varphi^t\|_{2s} := \max \{ \|\varphi_A^t\|_{2s}, \|\varphi_B^t\|_{2s} \} \quad (123)$$

$$\|v\|_{2r} := \max \{ \|v_A\|_{2r}, \|v_B\|_{2r}, \|v_{AB}\|_{2r} \} \quad (124)$$

and plug it into the equation above.

$$\begin{aligned} |\dot{\Omega}(t)| &\leq \|\varphi^t\|_{2s} \|v\|_{2r} \left\{ \left(6 + 3\frac{M}{N+M}\right) \frac{N}{N+M} \omega^{\varphi_A^t} \right. \\ &\quad \left. + \left(6 + 3\frac{N}{N+M}\right) \frac{M}{N+M} \omega^{\varphi_B^t} \right. \\ &\quad \left. + \frac{4}{N+M} + \frac{1}{N+M} \right\} \\ &\leq 9 \|\varphi^t\|_{2s} \|v\|_{2r} \left\{ (\Omega_A(t) + \Omega_B(t)) + \frac{1}{N+M} \right\} \\ &\leq C^{\varphi^t} \Omega(t) + \frac{C^{\varphi^t}}{N+M} \end{aligned} \quad (125)$$

with $C^{\varphi^t} := 9 \|\varphi^t\|_{2s} \|v\|_{2r}$. In this estimate, we replace the prefactors of $\omega^{\varphi_A^t}$ and $\omega^{\varphi_B^t}$, containing N and M, with 1, moreover, we apply (112).

Finally, we can take advantage of the Grönwall Lemma leading to the wanted final result by using (42)

$$\Omega(t) \leq e^{\int_0^t C^{\varphi^s} ds} \left(\Omega(0) + \frac{1}{N+M} \int_0^t C^{\varphi^s} e^{-\int_0^s C^{\varphi^\tau} d\tau} ds \right). \quad (126)$$

Never mind, in which order we apply the mean field limit, either $N \rightarrow \infty$ and then $M \rightarrow \infty$ or the other way round, we will in both cases get the same result: If $\Omega(0)$ converges in the mean field limit to 0 then also $\Omega(t)$ goes to 0. As before, the behavior due to the convergence of the sequence $\{\Omega_{N+M}(t)\}_{N+M \in \mathbb{N}}$ depends on the constant C^{φ^t} being independent of the number of particles. It even converges uniformly in $t \in [0, T]$ if $T < \infty$. If C^{φ^t} has compact support with respect to t and hence $\int_0^T \|\varphi^t\|_{2s} < \infty$ the ratio of bad particles converges for all times $t \in \mathbb{R}_0^+$ to 0 in the mean field limit. This follows from the same discussion as in section 3.4.6. Finally, these estimates manifest the Hartree equations which were heuristically derived in section 5.2 for the same arguments given in 3.4.4.

6.3 Conclusion

To conclude, if we start with a small amount of bad bosons in a system of two different types, where pair interaction occurs between all pairs of particles, then the fraction of bad particles can be neglected in the mean field limit for at most all finite times. Neither the interaction between two particles of the same species, nor the interaction between two different types can drastically increase the number of bad particles and that is the reason why we can neglect all kinds of correlations. Consequently (almost) product states keep their structure in the mean field limit for all times t .

6.4 Used computations

In this section, we list all the missing computations from the last section.

With a view to the determination of $|\dot{\Omega}(t)|$ we start with the following operator norm

$$\begin{aligned}
& \left\| p_1^{\varphi_A^t} \left(V_{AB}(\cdot - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right) (\cdot) \right)^2 p_1^{\varphi_A^t} \right\|_{op} \\
& \leq \sup_{x_{N+1} \in \mathbb{R}^3} \sup_{\|\phi\|_2=1} \left\| p_1^{\varphi_A^t} \left(V_{AB}(\cdot - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right) (\cdot) \right)^2 p_1^{\varphi_A^t} \phi \right\|_2 \\
& = \sup_{x_{N+1} \in \mathbb{R}^3} \sup_{\|\phi\|_2=1} \left| \langle \phi | \varphi_A^t \rangle \left\langle \varphi_A^t \left| \left(V_{AB}(\cdot - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right) (\cdot) \right)^2 \right| \varphi_A^t \right\rangle^2 \langle \varphi_A^t | \phi \rangle \right|^{\frac{1}{2}} \\
& = \sup_{x_{N+1} \in \mathbb{R}^3} \sup_{\|\phi\|_2=1} \left\| p_1^{\varphi_A^t} \phi \right\|_2 \left\langle \varphi_A^t \left| V_{AB}^2(\cdot - x_{N+1}) \right. \right. \\
& \quad \left. \left. - 2V_{AB}(\cdot - x_{N+1}) \left(V_{AB} * |\varphi_B^t|^2 \right) (\cdot) \right. \right. \\
& \quad \left. \left. + \left(V_{AB} * |\varphi_B^t|^2 \right)^2 (\cdot) \right| \varphi_A^t \right\rangle \\
& \leq \left\| p_1^{\varphi_A^t} \right\|_{op} \left\{ \sup_{x_{N+1} \in \mathbb{R}^3} \left| \langle \varphi_A^t | V_{AB}^2(\cdot - x_{N+1}) | \varphi_A^t \rangle \right| \right. \\
& \quad \left. + 2 \sup_{x_{N+1} \in \mathbb{R}^3} \left| \langle \varphi_A^t | V_{AB}(\cdot - x_{N+1}) \left(V_{AB} * |\varphi_B^t|^2 \right) (\cdot) | \varphi_A^t \rangle \right| \right. \\
& \quad \left. + \sup_{x_{N+1} \in \mathbb{R}^3} \left| \langle \varphi_A^t | \left(V_{AB} * |\varphi_B^t|^2 \right)^2 | \varphi_A^t \rangle \right| \right\} \\
& \leq \sup_{x_{N+1} \in \mathbb{R}^3} \left\| (\varphi_A^t)^2 \right\|_s \left\| V_{AB}^2(\cdot - x_{N+1}) \right\|_r \\
& \quad + 2 \sup_{x_{N+1} \in \mathbb{R}^3} \left\| (\varphi_A^t)^2 \right\|_s \left\| V_{AB}(\cdot - x_{N+1}) \left(V_{AB} * |\varphi_B^t|^2 \right) (\cdot) \right\|_r \\
& \quad + \left\| (\varphi_A^t)^2 \right\|_s \left\| \left(V_{AB} * |\varphi_B^t|^2 \right)^2 \right\|_r \\
& \leq \|\varphi_A^t\|_{2s}^2 \left\{ \|V_{AB}\|_{2r}^2 + 2 \sup_{x_{N+1} \in \mathbb{R}^3} \|V_{AB}(\cdot - x_{N+1})\|_{2r} \|V_{AB} * |\varphi_B^t|^2\|_{2r} + \left\| V_{AB} * |\varphi_B^t|^2 \right\|_{2r}^2 \right\} \\
& \leq \|\varphi_A^t\|_{2s}^2 \left\{ \|V_{AB}\|_{2r}^2 + 2 \|V_{AB}\|_{2r} \|V_{AB}\|_{2r} \left\| |\varphi_B^t|^2 \right\|_1 + \|V_{AB}\|_{2r}^2 \left\| |\varphi_B^t|^2 \right\|_1^2 \right\} \\
& \leq 4 \|\varphi_A^t\|_{2s}^2 \|V_{AB}\|_{2r}^2. \tag{127}
\end{aligned}$$

Here we used some Hölder estimates and Young's inequality. In addition, we profited by the normalization of the one-particle state φ_B^t .

Moreover, we continue with the estimate of term B)

$$\begin{aligned}
& \left| \left\langle \left\langle \Psi_{AB}^t \left| p_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} \left(V_{AB}(x_1 - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right)(x_1) \right) q_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \left| \Psi_{AB}^t \right\rangle \right\rangle \right| \\
&= \left| \left\langle \left\langle \Psi_{AB}^t \left| p_1^{\varphi_A^t} p_{N+1}^{\varphi_B^t} V_{AB}(x_1 - x_{N+1}) q_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \left| \Psi_{AB}^t \right\rangle \right\rangle \right| \\
&= \left| \left\langle \left\langle \Psi_{AB}^t \left| \frac{1}{N} \sum_{k=1}^N p_k^{\varphi_A^t} p_{N+1}^{\varphi_B^t} V_{AB}(x_k - x_{N+1}) q_k^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \left| \Psi_{AB}^t \right\rangle \right\rangle \right| \\
&\leq \left\| \frac{1}{N} \sum_{k=1}^N q_k^{\varphi_A^t} V_{AB}(x_k - x_{N+1}) p_k^{\varphi_A^t} p_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2 \left\| q_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2 \\
&= \left\{ \sum_{(k \neq l)=1}^N \left\langle \left\langle \Psi_{AB}^t \left| p_k^{\varphi_A^t} p_{N+1}^{\varphi_B^t} V_{AB}(x_k - x_{N+1}) q_k^{\varphi_A^t} q_l^{\varphi_A^t} V_{AB}(x_l - x_{N+1}) p_l^{\varphi_A^t} p_{N+1}^{\varphi_B^t} \left| \Psi_{AB}^t \right\rangle \right\rangle \right. \right. \\
&\quad \left. \left. + \sum_{k=1}^N \left\| q_k^{\varphi_A^t} V_{AB}(x_k - x_{N+1}) p_k^{\varphi_A^t} p_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2^2 \right\}^{\frac{1}{2}} \cdot \frac{\sqrt{\omega^{\varphi_B^t}}}{N} \\
&\leq \left\{ \sum_{(k \neq l)=1}^N \left\| V_{AB}(x_k - x_{N+1}) p_k^{\varphi_A^t} p_{N+1}^{\varphi_B^t} q_l^{\varphi_A^t} \Psi_{AB}^t \right\|_2 \left\| V_{AB}(x_l - x_{N+1}) p_l^{\varphi_A^t} p_{N+1}^{\varphi_B^t} q_k^{\varphi_A^t} \Psi_{AB}^t \right\|_2 \right. \\
&\quad \left. + \sum_{k=1}^N \left\| q_k^{\varphi_A^t} \right\|_{op} \left\| V_{AB}(x_k - x_{N+1}) p_k^{\varphi_A^t} p_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2^2 \right\}^{\frac{1}{2}} \cdot \frac{\sqrt{\omega^{\varphi_B^t}}}{N} \\
&\stackrel{(90)}{\leq} \frac{1}{N} \left\{ \sum_{(k \neq l)=1}^N \|\varphi_A^t\|_{2s}^2 \|V_{AB}\|_{2r}^2 \omega^{\varphi_A^t} + \sum_{k=1}^N \|\varphi_A^t\|_{2s}^2 \|V_{AB}\|_{2r}^2 \right\}^{\frac{1}{2}} \sqrt{\omega^{\varphi_B^t}} \\
&= \|\varphi_A^t\|_{2s} \|V_{AB}\|_{2r} \frac{1}{N} \left\{ (N^2 - N) \omega^{\varphi_A^t} + N \right\}^{\frac{1}{2}} \sqrt{\omega^{\varphi_B^t}} \\
&\leq \|\varphi_A^t\|_{2s} \|V_{AB}\|_{2r} \sqrt{\omega^{\varphi_A^t} + \frac{1}{N}} \sqrt{\omega^{\varphi_B^t}} \\
&\leq \frac{1}{2} \|\varphi_A^t\|_{2s} \|V_{AB}\|_{2r} \left(\omega^{\varphi_A^t} + \omega^{\varphi_B^t} + \frac{1}{N} \right) \tag{128}
\end{aligned}$$

where we used that $\sqrt{ab} \leq \frac{1}{2}(a+b)$ holds true $\forall a, b \in \mathbb{R}_0^+$ and $\frac{1}{r} + \frac{1}{s} = 1$.

Last but not least, we treat the term C)

$$\begin{aligned}
& \left| \left\langle \left\langle \Psi_{AB}^t \left| p_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \left(V_{AB}(x_1 - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right)(x_1) \right) q_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \left| \Psi_{AB}^t \right\rangle \right\rangle \right| \\
&\leq \left\| q_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2 \left\| \left(V_{AB}(x_1 - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right)(x_1) \right) p_1^{\varphi_A^t} q_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2 \\
&\leq \left\| q_1^{\varphi_A^t} \right\|_{op} \left\| q_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2 \left\| p_1^{\varphi_A^t} \left(V_{AB}(\cdot - x_{N+1}) - \left(V_{AB} * |\varphi_B^t|^2 \right)(\cdot) \right)^2 p_1^{\varphi_A^t} \right\|_{op}^{\frac{1}{2}} \left\| q_{N+1}^{\varphi_B^t} \Psi_{AB}^t \right\|_2 \\
&\leq 2 \|\varphi_A^t\|_{2s} \|V_{AB}\|_{2r} \omega^{\varphi_B^t}. \tag{129}
\end{aligned}$$

Here we used the Hölder inequality and the already computed inequality (127).

Part IV

Outlook

7 Time Evolution of Two Orthogonal States in One Bosonic System

In the second part, we introduced a method which permits us to determine the behavior of an N -particle bosonic system with good and bad bosons of one type in which pair interaction takes place between all particles. Furthermore, the third part concentrates on a mixture of two different kinds of bosons. In the following, we would like to give an outlook on another possible mixture of one type of bosons in two different good states. More detailed, for the experiment, we prepare separately one species of particles in two different eigenstates φ and χ which are without loss of generality perpendicular to each other. Beyond, we assume that the number of bad particles in each system is small compared to the corresponding particle number. Then, we mix the systems up and ask again the question: How does the number of bad particles evolve in time, when we allow pair interaction?

At first glance, this problem seems to be similar to that issue considered in the third part, but what is new is the fact that we cannot exactly determine which boson is in which state due to the bosonic character of the particles. Therefore, the wave function of all particles has to be symmetric under the exchange of bosons in the same state as well as under the exchange of particles in different states. Moreover, in this case, bad particles are those which are neither in the state φ nor in the state χ .

In this part, we just would like to give an outlook, concerning the described physical problem. Therefore, we keep the computations short, rather we would like to point out the difficulties which appear by following the strategy of the counting method. Additionally, we neglect in our notation the time dependence.

7.1 General description of the bosonic system

Let us introduce some notation. In total, we treat $N+M$ bosons, where N particles are in the system which we prepared to be in the state φ and where M particles are in the other state. The $N+M$ -particle states have to fulfill

$$\Psi_{N+M}(x_1, \dots, x_i, \dots, x_j, \dots, x_{N+M}) = \Psi_{N+M}(x_1, \dots, x_j, \dots, x_i, \dots, x_{N+M}) \quad (130)$$

with $1 \leq i, j \leq N+M$. In order to emphasize it again, since we treat a bosonic system with only one type of particles in two different states, we have to take into consideration that the $N+M$ -particle state is additional symmetric under the exchange of particles in the different states. The hamilton for the system looks just like in part II

$$H_{N+M} = \sum_{j=1}^{N+M} (-\Delta_j) + \sum_{j=1}^{N+M} A^t(x_j) + \sum_{1 \leq j < k \leq N} V(x_j - x_k) \quad (131)$$

where A^t is some external potential and V_{N+M} is the spherical symmetric pair interaction. Beyond, the symmetric and normalized product state in this case reads as

$$\Psi_{N+M} = \frac{1}{\sqrt{\binom{N+M}{N}}} \left(\prod_{j=1}^N \varphi(x_j) \prod_{k=N+1}^{N+M} \chi(x_k) \right)_{sym}. \quad (132)$$

Notice, the normalized states φ and χ are perpendicular to each other and therefore only the diagonal term contribute to the normalization of Ψ_{N+M} . Additionally, the reduced one-particle density matrix of the N+M-particle state given above, has the following structure

$$\mu^{\Psi_{N+M}}(x_j) = \frac{N}{N+M} |\varphi(x_j)\rangle \langle \varphi(x_j)| + \frac{M}{N+M} |\chi(x_j)\rangle \langle \chi(x_j)|. \quad (133)$$

In comparison to part II, we call Ψ_{N+M} a product state of two orthogonal allowed states, because for $M = 0$ the expression above equals the reduced one-particle density matrix for only one state, as it is in (6).

Next comes the deviation of the Hartree equations for the two different states. Here, we use the Euler-Lagrange formalism to minimize the total energy of the system which is in the product state (132). Further, we want to stress that the following calculation is correct, however, there are a few physical aspects which are neglected in this case. More details are mentioned in section 3.3. The total energy looks like

$$\begin{aligned} \langle \langle \Psi_{N+M} | H_{N+M} | \Psi_{N+M} \rangle \rangle = & \frac{1}{\binom{N+M}{N}} \left\{ N \langle \varphi(x) | (-\Delta_x) | \varphi(x) \rangle + M \langle \chi(x) | (-\Delta_x) | \chi(x) \rangle \right. \\ & + N \langle \varphi(x) | A^t(x) | \varphi(x) \rangle + M \langle \chi(x) | A^t(x) | \chi(x) \rangle \\ & + \binom{N}{2} \langle \varphi(x)\varphi(y) | V(x-y) | \varphi(x)\varphi(y) \rangle \\ & + \binom{M}{2} \langle \chi(x)\chi(y) | V(x-y) | \chi(x)\chi(y) \rangle \\ & + N \cdot M \langle \varphi(x)\chi(y) | V(x-y) | \varphi(x)\chi(y) \rangle \\ & \left. + N \cdot M \langle \varphi(x)\chi(y) | V(x-y) | \chi(x)\varphi(y) \rangle \right\}. \quad (134) \end{aligned}$$

The numerical factors appear due to the bosonic character of the considered system. Moreover, we assume that φ is a function vanishing at infinity and therefore we can write

$$\begin{aligned} \langle \varphi(x) | -\Delta_x | \varphi(x) \rangle &= \int \varphi^* (-\Delta_x) \varphi(x) dx \\ &= \int (\nabla_x \varphi)^* (x) (\nabla_x \varphi) (x) dx = \|\nabla \varphi\|_2^2. \quad (135) \end{aligned}$$

The Euler-Lagrange formalism with additional condition that φ and χ are normalized to one gives us a function φ , or χ respectively, which minimizes the functional $F = F(\varphi^*, (\nabla \varphi)^*, x)$ which is defined as

$$\begin{aligned} \int F(\varphi^*, (\nabla \varphi)^*, x) dx &= \langle \langle \Psi_{N+M} | H_{N+M} | \Psi_{N+M} \rangle \rangle \\ &\quad - \lambda \frac{N}{\binom{N+M}{N}} \left(\|\varphi\|_2^2 - 1 \right) - \tau \frac{M}{\binom{N+M}{M}} \left(\|\chi\|_2^2 - 1 \right). \quad (136) \end{aligned}$$

We compute the variation with respect to φ^* because afterwards, we can immediately read off the Hartree equation for φ . Because of the Euler-Lagrange formalism

$$\nabla_x \left(\frac{\delta F}{\delta (\nabla_x \varphi)^*} \right) - \frac{\delta F}{\delta \varphi^*} = 0 \quad (137)$$

is valid. The single expressions read as

$$\nabla_x \left(\frac{\delta F}{\delta (\nabla_x \varphi)^*} \right) = \frac{N}{\binom{N+M}{N}} \Delta_x \varphi(x) \quad (138)$$

as well as

$$\begin{aligned} \frac{\delta F}{\delta \varphi^*} = \frac{N}{\binom{N+M}{N}} & \left\{ A^t(x) \varphi(x) + (N-1) \int \varphi^*(y) V(x-y) \varphi(y) dy \cdot \varphi(x) \right. \\ & + M \int \chi^*(y) V(x-y) \chi(y) dy \cdot \varphi(x) \\ & \left. + M \int \chi^*(y) V(x-y) \varphi(y) dy \cdot \chi(x) - \lambda \varphi(x) \right\}. \end{aligned} \quad (139)$$

The variation with respect to φ^* of the summand $\langle \varphi \varphi | V | \varphi \varphi \rangle$ produces a factor of 2 because there, we handle with a $(\varphi^*)^2$.

Note, the Lagrange multiplier λ represents the energy e_φ of one particle in the state φ and due to the Schrödinger equation, we can write

$$\lambda \varphi = e_\varphi \varphi = i \partial_t \varphi \quad (140)$$

Therefore the equation (137) yields to

$$\begin{aligned} i \partial_t \varphi(x) = & \left\{ -\Delta_x + A^t(x) + (N-1) \left(V * |\varphi|^2 \right) (x) + M \left(V * |\chi|^2 \right) (x) \right\} \cdot \varphi(x) \\ & + M \left(V * (\chi^* \varphi) \right) (x) \cdot \chi(x) \end{aligned} \quad (141)$$

$$= h^\varphi(x) \varphi(x) + M a(x) \chi(x) \quad (142)$$

which is the Hartree equation for a bosonic system with one type of particles but two different orthogonal states, with $a(x) = \left(V * (\chi^* \varphi) \right) (x)$. We know already the first summand of the equality from section 5.2, compare (108), which represents the Hartree equation for two different species of particles. However, the additional part can be interpreted as a term of exchange. It has its origin from the property that the N+M-particle state has to be symmetric in all variables. We rewrite it in a more obvious way

$$M |\chi(x)\rangle \langle \chi(y) | V(x-y) | \varphi(y)\rangle \quad (143)$$

The initial state of our considered particle is φ . Because of the interaction, the particle immediately takes on the χ -properties and ends up in the state χ , i.e. the particle jumps from a state φ into a state χ . The prefactor M denotes the number of possibilities in which the original state φ can transfer to.

For completion, we also add the Hartree equation for the state χ , which follows from (141) by interchanging χ and φ as well as N and M.

$$\begin{aligned} i \partial_t \chi(x) = & \left\{ -\Delta_x + A^t(x) + (M-1) \left(V * |\chi|^2 \right) (x) + M \left(V * |\varphi|^2 \right) (x) \right\} \cdot \chi(x) \\ & + M \left(V * (\varphi^* \chi) \right) (x) \cdot \varphi(x) \end{aligned} \quad (144)$$

$$= h^\chi(x) \chi(x) + N a^*(x) \varphi(x) \quad (145)$$

7.2 Application of the strategy of counting bad particles

Now, we have all tools in order to apply the method of counting bad particles. As already mentioned, bad particles are those which are neither in the state φ nor in the state χ , therefore the projector is given as

$$q = 1 - p^\varphi - p^\chi. \quad (146)$$

We consider a system with $N+M$ bosons in an arbitrary initial state Ψ_{N+M} such that we can assume that the number of bad particles is small compared to the total number. In the following, we compute the time derivative of the ratio of bad particles $\Omega = \langle\langle \Psi | q | \Psi \rangle\rangle$, where we use the Schrödinger equation $i\partial_t \Psi_{N+M} = H_{N+M} \Psi_{N+M}$,

$$\begin{aligned} \dot{\Omega} &= \left(\langle\langle \Psi_{N+M} | \dot{q} | \Psi_{N+M} \rangle\rangle \right) \\ &= i \langle\langle \Psi_{N+M} | [H_{N+M}, q] | \Psi_{N+M} \rangle\rangle + \langle\langle \Psi_{N+M} | \dot{q} | \Psi_{N+M} \rangle\rangle. \end{aligned} \quad (147)$$

To continue, we calculate \dot{p}^φ as well as \dot{p}^χ

$$\begin{aligned} \dot{p}^\varphi &= |\dot{\varphi}\rangle \langle\varphi| + |\varphi\rangle \langle\dot{\varphi}| \\ &\stackrel{(142)}{=} -i \left(h^\varphi(x) |\varphi\rangle \langle\varphi| + M a(x) |\chi\rangle \langle\varphi| \right) + i \left(|\varphi\rangle \langle\varphi| h^\varphi(x) + M |\varphi\rangle \langle\chi| a^*(x) \right) \\ &= -i [h^\varphi, p^\varphi] - iM \left(a(x) |\chi\rangle \langle\varphi| - |\varphi\rangle \langle\chi| a^*(x) \right). \end{aligned} \quad (148)$$

Consequently, it results

$$\dot{p}^\chi = -i [h^\chi, p^\chi] - iN \left(a^*(x) |\varphi\rangle \langle\chi| - |\chi\rangle \langle\varphi| a(x) \right). \quad (149)$$

To sum up, the calculation yields to

$$\begin{aligned} \dot{\Omega}(t) &= iN \left\{ \langle\langle \Psi_{N+M} \left| \left[V_{N+M}(x_1 - x_2) - \left(V_{N+M} * |\varphi|^2 \right)(x_1), q_1 \right] \right| \Psi_{N+M} \rangle\rangle \right. \\ &\quad + \langle\langle \Psi_{N+M} | \left(V_{N+M} * (\varphi^* \chi) \right)(x_1) |\chi(x_1)\rangle \langle\varphi(x_1)| \\ &\quad \quad \quad \left. - |\varphi(x_1)\rangle \langle\chi(x_1)| \left(V_{N+M} * (\chi^* \varphi) \right)(x_1) | \Psi_{N+M} \rangle\rangle \right\} \\ &+ iM \left\{ \langle\langle \Psi_{N+M} \left| \left[V_{N+M}(x_1 - x_2) - \left(V_{N+M} * |\chi|^2 \right)(x_1), q_1 \right] \right| \Psi_{N+M} \rangle\rangle \right. \\ &\quad + \langle\langle \Psi_{N+M} | \left(V_{N+M} * (\chi^* \varphi) \right)(x_1) |\varphi(x_1)\rangle \langle\chi(x_1)| \\ &\quad \quad \quad \left. - |\chi(x_1)\rangle \langle\varphi(x_1)| \left(V_{N+M} * (\varphi^* \chi) \right)(x_1) | \Psi_{N+M} \rangle\rangle \right\} \\ &+ i \langle\langle \Psi_{N+M} \left| \left[V_{N+M}(x_1 - x_2) - \left(V_{N+M} * |\varphi|^2 \right)(x_1), p_1^\varphi \right] \right| \Psi_{N+M} \rangle\rangle \\ &+ i \langle\langle \Psi_{N+M} \left| \left[V_{N+M}(x_1 - x_2) - \left(V_{N+M} * |\chi|^2 \right)(x_1), p_1^\chi \right] \right| \Psi_{N+M} \rangle\rangle. \end{aligned} \quad (150)$$

In the following, we take the term with the prefactor N into account. As before, we insert again identities, $1 = q_j + p_j^\varphi + p_j^\chi$ with $j \in \{1, 2\}$. Therefore, the commutator reads as

$$\left[(q_1 + p_1^\varphi + p_1^\chi) (q_2 + p_2^\varphi + p_2^\chi) \left(V_{N+M}(x_1 - x_2) - \left(V_{N+M} * |\varphi|^2 \right)(x_1) \right), q_1 (q_2 + p_2^\varphi + p_2^\chi) \right] \quad (151)$$

which yields at all to $2 \cdot 3 \cdot 3 \cdot 3 = 54$ terms. Due to the symmetric character of Ψ_{N+M} and the commutator almost half of the summands cancel out. For the appliance of the Grönwall Lemma,

we need to estimate the remaining terms such that they are affine with respect to Ω . Nevertheless, there exist terms whose assessment yields only to $\sqrt{\Omega}$. We infer from $0 \leq \Omega \leq 1$ which holds true by definition that $\sqrt{\Omega} \geq \Omega$ is valid and as a consequence we cannot use Grönwall's Lemma to create an upper bound for the ratio of bad particles. Let us have a look at one diverging term which appears

$$\begin{aligned}
 & \left\langle \left\langle \Psi_{N+M} \left| p_1^\varphi p_2^\chi \left(V_{N+M}(x_1 - x_2) - \left(V_{N+M} * |\varphi|^2 \right) (x_1) \right) q_1 p_2^\varphi \right| \Psi_{N+M} \right\rangle \right\rangle \\
 &= \left\langle \left\langle \Psi_{N+M} \left| p_1^\varphi p_2^\chi V_{N+M}(x_1 - x_2) q_1 p_2^\varphi \right| \Psi_{N+M} \right\rangle \right\rangle \\
 &\leq \sqrt{\Omega} \|p_1^\varphi p_2^\chi \Psi_{N+M}\|_2 \left\langle \varphi(x_1) \left| V_{N+M} * (\chi^* \varphi)^2 (x_1) \right| \varphi(x_1) \right\rangle^{\frac{1}{2}} \\
 &\leq \|\varphi\|_{2s} \|V_{N+M}\|_{2r} \sqrt{\Omega}.
 \end{aligned} \tag{152}$$

Here we used the following estimate

$$\begin{aligned}
 & \left\langle \varphi(x_1) \left| V_{N+M} * (\chi^* \varphi)^2 (x_1) \right| \varphi(x_1) \right\rangle \\
 &\leq \|\varphi\|_{2s}^2 \|V_{N+M} * (\chi^* \varphi)\|_{2r}^2 \\
 &\leq \|\varphi\|_{2s}^2 \|V_{N+M}\|_{2r}^2 \|\chi^* \varphi\|_1^2 \\
 &\leq \|\varphi\|_{2s}^2 \|V_{N+M}\|_{2r}^2 \|\chi\|_2^2 \|\varphi\|_2^2 \\
 &= \|\varphi\|_{2s}^2 \|V_{N+M}\|_{2r}^2
 \end{aligned} \tag{153}$$

with the Hölder condition $\frac{1}{r} + \frac{1}{s} = 1$. To sum up, with the prefactor N and the order $\frac{1}{N+M}$ of the potential we rest at

$$\begin{aligned}
 & \left\langle \left\langle \Psi_{N+M} \left| p_1^\varphi p_2^\chi \left(V_{N+M}(x_1 - x_2) - \left(V_{N+M} * |\varphi|^2 \right) (x_1) \right) q_1 p_2^\varphi \right| \Psi_{N+M} \right\rangle \right\rangle \\
 &\leq \|\varphi\|_{2s} \|v\|_{2r} \frac{N}{N+M} \sqrt{\Omega}.
 \end{aligned} \tag{154}$$

It is not possible to do further estimates from above such that this formula becomes proportional to Ω and the mean field limit $N \rightarrow \infty$ and afterwards $M \rightarrow \infty$ converges. Thus, we cannot predict the behavior of this expression in the mean field limit. Consequently, we fail to determine the time evolution of Ω , when we follow the strategy of part II.

Furthermore, we would like to give a heuristic argument why the $\sqrt{\Omega}$ -dependency leads to an ordinary differential equation whose solution does not converge to 0 in the mean field limit. In consequence, under these assumptions we cannot take for granted that product states keep their characteristics in such a bosonic system.

Moreover, the time derivative of the ratio of bad particles is expected to have the structure

$$\left| \dot{\Omega}(t) \right| \leq a(t) \sqrt{\Omega} + b(t) \Omega + \mathcal{O} \left(\frac{1}{N}, \frac{1}{M}, \frac{1}{N+M} \right) \tag{155}$$

Since $0 \leq \Omega \leq 1$ is valid, also $\Omega \leq \sqrt{\Omega}$ holds true. Besides, we neglect the additional terms of order $\frac{1}{N}$, $\frac{1}{M}$ and $\frac{1}{N+M}$. Further, the time dependent functions abbreviated with $a(t)$ and $b(t)$ are positive and finite for all times, because they replace products of norms, e.g. $\|\varphi\|_{2s}^2 \|v\|_{2r}^2$. Additionally, they are of order 1 with respect to the number of particles such that they converge for sure in the mean field limit $N \rightarrow \infty$ and $M \rightarrow \infty$ or vice versa. Therefore, we can compute

$$\left| \dot{\Omega}(t) \right| \leq \left(a(t) + b(t) \right) \sqrt{\Omega} \tag{156}$$

where the general solution can be estimated from above via

$$|\Omega(t)| = \Omega(t) \leq \left(\frac{1}{2} \int_0^t (a(\tau) + b(\tau)) d\tau + \sqrt{\Omega(0)} \right)^2. \quad (157)$$

The proof for this is equivalent to the proof we gave for the Grönwall Lemma in chapter 2.

If we apply the mean field limit on (157), only $\Omega(0)$ converges to 0 according to the assumption, the integral remains untouched. Due to the fact that a and b are positive functions, the upper bound of $\Omega(t)$ increases generally in time.

To conclude, estimates, which give a $\sqrt{\Omega}$ -dependency destroy the convergence of the upper bound to 0 and therefore we arrive at three possible solutions. Either we can find a lower bound of $\Omega(t)$ which also predicts that $\Omega(t)$ increases with growing time, or the heuristic estimate above is not strict enough, or the method of counting bad particles fails in this case. The former leads to the result that the structure of the state Ψ_{N+M}^t would be destroyed and for that reason we cannot infer from

$$\mu^{\Psi_{N+M}}(x_j) \xrightarrow{N, M \rightarrow \infty} \frac{N}{N+M} |\varphi(x_j)\rangle \langle \varphi(x_j)| + \frac{M}{N+M} |\chi(x_j)\rangle \langle \chi(x_j)| \quad (158)$$

that this holds for all times. As a consequence, we cannot deduce the time evolution of (almost) product states.

7.3 Introduction of quasi-particles

In order to get a solution for this problem, one could try to introduce quasi-particles consisting of two bosons, one in state φ and the other in state χ . Consequently, one has to take for granted that the particle numbers of the different states N and M are equal. Moreover it should be clarified how the product state as well as the Hartree equation looks like in this case. Finally, one has to identify bad particles and estimate the time derivative of the ratio of bad particles from above, in order to apply the Grönwall Lemma.

We assume that the quasi-particles are in a superposition of the two normalized states φ and χ . Now, we have to ask the question, how to define the projector q and consequently the counting measure. In the following, we deal with two possibilities. On the one hand, we declare all bosons as bad particles which are not exactly in the superposition $\frac{1}{\sqrt{2}}(\varphi + \chi)$. While, on the other hand, we treat those particles as bad particles which are neither in the state φ nor in the state χ nor in any superposition of both of them. This consideration yields to the two different starting points

$$q^{\varphi+\chi} := 1 - p^{\varphi+\chi} = 1 - \frac{1}{2} |\varphi + \chi\rangle \langle \varphi + \chi| = 1 - \frac{1}{2} \left(|\varphi\rangle \langle \varphi| + |\varphi\rangle \langle \chi| + |\chi\rangle \langle \varphi| + |\chi\rangle \langle \chi| \right) \quad (159)$$

$$q^{\varphi, \chi} := 1 - p^\varphi - p^\chi = 1 - |\varphi\rangle \langle \varphi| - |\chi\rangle \langle \chi|. \quad (160)$$

First of all, we take the definition (159) into account. The Hartree equation looks like

$$i\partial_t (\varphi(x) + \chi(x)) = \left\{ -\Delta_x + A(x) + (N-1) \left(V_N * |\varphi + \chi|^2 \right) (x) \right\} (\varphi(x) + \chi(x)). \quad (161)$$

Notice, in this case, we cannot determine the dynamics of one single state.

However, we already discussed this circumstance in detail in part II. Here, in this description, we have to replace the former φ by the superposition $\frac{1}{\sqrt{2}}(\varphi + \chi)$ and the strategy of counting bad particles works perfectly. It ends up with the result that (almost) product states remain (almost) product states, as we have shown.

Nevertheless, the model which we use here is too easy, since we just concentrate on the superposition $\frac{1}{\sqrt{2}}(\varphi + \chi)$. In other words, we join two particles in the state φ and χ together to make one new boson in the superposition and the strategy goes through. Therefore, the simplification of our original bosonic system consisting of two distinguishable states φ and χ is too strong.

What about superpositions with different weights of the state φ and χ ? In order to see what happens, we compute

$$\langle \alpha\varphi + \beta\chi | q^{\varphi+\chi} | \alpha\varphi + \beta\chi \rangle = \frac{1}{2} (1 - 2 \cdot \text{Re}[\alpha^* \beta]) \quad (162)$$

where $\alpha, \beta \in \mathbb{C}$ with the condition $|\alpha|^2 + |\beta|^2 = 1$ and where $\text{Re}[z]$ denotes the real part of $z \in \mathbb{C}$. Therefore all bosons in states with different weights are counted as bad particles. Especially, the pure one-particle states φ as well as χ are declared as bad particles. To sum up, the $q^{\varphi+\chi}$ as defined in (159) contradicts to our original model, where a bad particle is a boson which is neither in the state φ nor in the state χ .

We go on with the other definition of $q^{\varphi \cdot \chi}$ in (160). Here, all quasi-particles which are in some superposition of φ and χ are good particles. In order to stay more heuristic, we go back to calculation (152). There, we consider one term which appears in the calculation of the time derivative of the ratio of bad particles, if we choose the projector as in (160). The mean field interaction always drops out because of the orthogonality of φ and χ and we receive an upper bound being proportional to $\sqrt{\Omega}$. As we already discussed above, this dependency leads to a diverging ratio of bad particles. Hence, we get no result to the given problem.

To conclude, the introduction of quasi-particles is justified and leads to a discussion concerning the definition of the counting operator and the counting measure.

Part V

Conclusion

In general, we considered bosonic systems where spherical symmetric pair interaction occurs between all pairs of particles. Assuming that the reduced one-particle density matrix of the initial state which describes the whole system, takes on product structure in the mean field limit, we show that this also holds true for arbitrary times t .

At the beginning, we connected the convergence of the reduced one-particle density matrix in operator norm with the number of bad particles. Here, we assured that the reduced one-particle density matrix converges in the mean field limit to a one-particle state if and only if the number of bad bosons compared to the particle number goes to 0. Moreover, this is equivalent to the almost product structure of the initial state of the system. In order to emphasize it, in our consideration an almost product state behaves in the mean field limit as a product state. This does not work in L^2 -sense, since in that case, the notion of distance is too strong.

In part II, we worked on a system with one type of particles which move in some external potential. Since we would like to consider physical interesting systems, we have to rescale the pair interaction with one over the particle number, such that the energy is equally distributed on kinetic and potential energy as well as on the pair interaction. From the well known Schrödinger equation for the whole system, we derive the Hartree equation, which describes the dynamics of a one-particle state in the mean field of the remaining particles. According to the name, we deduced the mean field interaction of one single boson by the interaction with the distributed particles around. Note that we need the empirical distribution which can be measured and which illustrates the real experiment. Nevertheless, the law of large numbers as well as the rescaling of the pair interaction affirm that the theoretical distribution equals the empirical distribution for large particle numbers.

Afterwards, we estimated the time derivative of the ratio of bad particles from above in order to use Grönwall's Lemma at the end. This lemma tells us that, if one can give an upper bound of the derivative of a function which is affine to the function itself, then one can bound this function from above.

There is one problem, when we estimate the time derivative of the ratio of bad particles, the state of the whole system is unknown. Notwithstanding, we are familiar to its dynamics due to the Schrödinger equation and the behavior of the reduced one-particle density matrix at the beginning. Following the computation, we arrive at the commutator of the difference of the Hamiltonians of the whole system and the one-particle state and the projector counting bad particles. Here, we insert a few identities consisting of the projectors which project in the direction of the state which appears in the mean field limit of the reduced one-particle density matrix and its orthogonal counterpart. Consequently, we receive an amount of summands. Due to the symmetric character and the commutator, many terms cancel out. Three terms and their complex conjugate survive which can be estimated from above, such that they satisfy the condition for the Grönwall Lemma. Applying this lemma leads to an upper bound for the ratio of bad particles which vanishes in the mean field limit for finite times t . This is equivalent to the convergence of the reduced one-particle density matrix to a pure state at arbitrary finite times.

To conclude, although there is correlation between the particles in a system due to pair interaction, an (almost) non correlated state at the beginning keeps its structure in the mean field limit at least for finite times t .

In part III, we treated a system consisting of two different types of bosons, where pair interaction takes place between all bosons. Additionally to the Hartree equation in part II, we get a further interaction term, which describes the interaction with bosons of the other species. Similarly, we arrive at the result that (almost) product states remain (almost) product states in the mean field limit even if there is interaction and therefore the bosons influence each other.

Last but not least, we give a short outlook to a system with one type of bosons which are in two different states. In contrast to part III, there is a further term in the Hartree equation representing the exchange of particles into the other state. Here, our solution would be that the reduced one-particle density matrix does not converge in the mean field limit to a pure state. It is not known, if the method fails, or nature just behaves like this.

To conclude, we proved that initial (almost) product states keep their properties at any time in a system consisting of one or two different types of bosons with large particle numbers, where pair interaction occurs between all pairs of bosons.

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Eidesstattliche Erklärung

Ich erkläre hiermit, dass ich die vorliegende Arbeit selbständig angefertigt, alle Zitate als solche kenntlich gemacht sowie alle benutzten Quellen und Hilfsmittel angegeben habe.

(Datum)

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