

Mean-field approximations of fermionic  
systems

Näherungen fermionischer Systeme durch  
gemittelte Felder

Fynn Jerome Aschmoneit

19. Dezember 2013

Bachelorarbeit an der Fakultät für Physik der Ludwig-Maximilians  
Universität München

Betreuer: Prof. Dr. Peter Pickl, Prof. Dr. Immanuel Bloch



# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
<b>2</b>	<b>Scalings</b>	<b>3</b>
2.1	The mean-field Hamiltonian . . . . .	3
2.2	The semiclassical scale . . . . .	4
2.3	Volume linear in $N$ . . . . .	8
<b>3</b>	<b>Derivation of the Hartree-Fock equations for fermionic systems</b>	<b>13</b>
3.1	The stationary Hartree-Fock equations . . . . .	13
3.2	Argument for a time dependent Hartree-Fock equation . . . . .	18
<b>4</b>	<b>An approach to a mean-field approximation</b>	<b>21</b>
4.1	The counting operator $\alpha$ . . . . .	22
4.2	The time derivative of $\alpha$ . . . . .	23
<b>5</b>	<b>Auxiliary calculations and examples</b>	<b>29</b>
<b>6</b>	<b>Bibliography</b>	<b>33</b>



# 1 Introduction

This thesis aims to give an introduction to the approximation of interacting fermionic systems by mean-field approximations.

The high quality of these approximations is experimentally proven and mean-field approximations are widely applied to simplify many-particle interactions. For example, electrons in metals whose energy is above the Fermi-level are assumed to move in some periodic potential (external potential generated by the nuclei) and a mean potential generated by other electrons (this model is used to describe the electric conductivity). Nevertheless, it is difficult to find a complete derivation of the validity of such approximations.

As fermions are antisymmetric with respect to particle exchange, a fermionic state is given by the normalized sum of all permutations of particles. This is described by a Slater determinant of  $N$  one-particle wave functions:

$$\Psi_N(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_n} \text{sgn}(\sigma) \prod_{j=1}^N \phi_j(x_{\sigma_j}) \quad (1.1)$$

$S_n$  describes all possible permutations of  $x_i$ ,  $i = 1, \dots, N$  and

$$\text{sgn}(\sigma) = \begin{cases} 1 & , \text{if } \sigma \text{ describes an even amount of permutations} \\ -1 & , \text{otherwise.} \end{cases}$$

The  $\phi_j$  are solutions of the Hartree-Fock equations.

A mean-field approximation is assumed to be valid if a fermionic system converges to the Slater determinant (1.1) in the mean-field limit  $N \rightarrow \infty$ , under the constraint of it converging for an initial state.

This thesis basically consists of three chapters: The chapter "Scalings" is concerned with finding a Hamiltonian which is still meaningful in the mean-field limit  $N \rightarrow \infty$ . I.e. neither its kinetic term nor its interaction term diverges with respect to the other one. The mean-field Hamiltonian is then derived for two different physical systems.

The chapter "Derivation of the Hartree-Fock equations for fermionic systems" explains the importance of solutions of the Hartree-Fock equations for mean-field approximations. Firstly, a derivation of the Hartree-Fock equations is given and secondly, an argument for the validity of dynamic Hartree-Fock equations is presented.

In chapter "An approach to a mean-field approximation", the method of the counting operator  $\alpha$  is introduced, which is applicable to either one of the two systems derived in "Scalings", using the dynamic Hartree-Fock equations presented in chapter "Derivation of the Hartree-Fock equations for fermionic systems". This chapter finishes with an outline of how to derive the proof of the validity of the mean-field approximation of the two systems described in chapter "Scalings".

To improve the readability, some calculations, derivations and examples are collected in the appendix "Auxiliary calculations and examples", p. 29.

## 2 Scalings

The Scaling of variables of a system is essential when observing a system in the limit of a parameter, if taking the limit of this parameter implied the divergence or annihilation of the quantity of interest.

In the case of mean-field limits of interacting systems, the kinetic energy and the interaction potential, the two quantities of interest, grow in some way with the particle number  $N$ . The scaling prevents either one of the quantities to diverge with respect to the other one as  $N \rightarrow \infty$ . It therefore provides, that the kinetic energy and the interaction potential are comparable in the mean-field limit, what is taken advantage of, when observing a mean-field approximation in its time evolution.

In this chapter, firstly, a set of coordinates is defined in such a way that the scaled Hamiltonian is applicable to describe a system in the mean-field limit. Secondly, the scaling parameters are determined for two systems of great physical interest: The first system resembles a Dirac-Sea, though not treated relativistically and neglecting negative energy states. It therefore describes the fermionic equivalent to a Bose-Einstein condensate and is applicable when the particle density increases with the number of particles, e.g. for large atoms. The other system is described by a model whose volume grows linearly in  $N$  and therefore, keeps its particle density constant. This model is applied for solids or big molecules.

The following estimates show that the kinetic energy in the first system grows a lot faster with  $N$  than the second system. This behaviour is due to the Fermi pressure, as because of the limited volume, the particles are confined to, higher energy states become occupied. Whereas for the second system exists some unity volume for every particle and therefore, the particles are not forced into higher states as the number of particles increases.

### 2.1 The mean-field Hamiltonian

In order to be able to compare the kinetic energy with the potential energy of a system in the mean-field limit ( $N \rightarrow \infty$ ), the coordinates ( $\underline{x}$ ), as well as the time  $t$ , need to be scaled in a way such that the kinetic energy and the interaction potential are of the same order in  $N$ . Let  $\tilde{\underline{x}}, \underline{x} \in \mathbb{R}^{3N}$  and  $\tilde{x}_i, x_i \in \mathbb{R}^3$  for  $i = 1, 2, \dots, N$ . Neglecting an external potential, the Hamiltonian for a system with the pairwise Coulomb interaction ( $e = 1$ ) reads as:

$$i\partial_{\tilde{t}}\tilde{\Psi}(\tilde{\underline{x}}, \tilde{t}) = -\sum_{i=1}^N \Delta_{\tilde{x}_i} \tilde{\Psi}(\tilde{\underline{x}}, \tilde{t}) + \sum_{1 \leq i < j \leq N} \frac{1}{\|\tilde{x}_i - \tilde{x}_j\|} \tilde{\Psi}(\tilde{\underline{x}}, \tilde{t}) \quad (2.1)$$

Here, and in the following, the norm  $\|\cdot\|$  denotes the 2-norm  $\|\cdot\|_2$ . With  $\epsilon_1, \epsilon_2 \in \mathbb{R}_+$ , a new set of coordinates is defined as:

$$\begin{aligned} t &= \epsilon_1 \tilde{t} \quad \text{and} \quad \underline{x} = \epsilon_2 \tilde{\underline{x}} \\ \tilde{\Psi}(\tilde{\underline{x}}, \tilde{t}) &\longrightarrow A\Psi\left(\frac{1}{\epsilon_2}\underline{x}, \frac{1}{\epsilon_1}t\right) \\ \partial_{\tilde{t}} &\longrightarrow \epsilon_1 \partial_t \quad \text{and} \quad \partial_{\tilde{\underline{x}}} \longrightarrow \epsilon_2 \partial_{\underline{x}} \end{aligned}$$

applying these transformations to the Hamiltonian (2.1), leads to the rescaled Hamiltonian in the coordinates  $(\underline{x}, t)$ :

$$i\epsilon_1 \partial_t \Psi(\underline{x}, t) = -\epsilon_2^2 \sum_{i=1}^N \Delta_{x_i} \Psi(\underline{x}, t) + \epsilon_2 \sum_{1 \leq i < j \leq N} \frac{1}{\|x_i - x_j\|} \Psi(\underline{x}, t) \quad (2.2)$$

As the terms above need to be adjustable in the order in  $N$ , the new coordinates  $(\underline{x}, t)$  need to depend on  $N$  themselves. Therefore, defining  $\epsilon_1 = N^a$  and  $\epsilon_2 = N^b$ , (2.2) can be written as:

$$i\partial_t \Psi(\underline{x}, t) = -N^{2b-a} \sum_{i=1}^N \Delta_{x_i} \Psi(\underline{x}, t) + N^{b-a} \sum_{1 \leq i < j \leq N} \frac{1}{\|x_i - x_j\|} \Psi(\underline{x}, t) \quad (2.3)$$

In the following, the kinetic energy and the interaction potential are estimated for two different systems. The parameters  $a, b$  are then identified, such that kinetic and interaction potential are of the same order in  $N$ .

## 2.2 The semiclassical scale

This chapter considers a system, which is comparable to the model of a three dimensional box, of constant volume  $V = L^3$ , which is successively filled with interacting fermions. If the fermions energies are close to their accessible ground state energies, this model could describe ground states of large atoms or white dwarfs (but these need a relativistic treatment as the Fermi energy, and therefore the Fermi velocity, is very big). The following calculation shows, that the kinetic energy and the interaction potential are of order  $\mathcal{O}(N^{\frac{5}{3}})$  and  $\mathcal{O}(N^2)$ , respectively.

For the estimate of the order of the kinetic energy in  $N$ , suppose, that the particles don't interact with each other, that the box is small enough to apply a periodic boundary condition and, that an external potential is neglected. This is equivalent to the free gas approximation, first described by Arnold Sommerfeld and Hans Bethe in [2]. Assuming  $\hbar = \frac{m}{2} = 1$ , the  $N$ -particle hamiltonian reads as:

$$-\sum_{j=1}^N \Delta_{x_j} \Psi(\underline{x}) = -\sum_{j=1}^N h^{(j)} \Psi(\underline{x}) = E\Psi(\underline{x})$$

, where  $h^{(j)}$  act on the one particle states  $\phi_j$ . Applying the periodic boundary condition, the constraints for the one particle states are:



$$\begin{aligned}
\phi(x_j) &= \phi(x_j^x, x_j^y, x_j^z) = \\
\phi(x_j^x + L, x_j^y, x_j^z) &= \phi(x_j^x, x_j^y + L, x_j^z) = \phi(x_j^x, x_j^y, x_j^z + L) \\
\text{and } \|\phi\| &= 1
\end{aligned}$$

Automatically, the N-particle wave function obeys the constraints, for as long as the one particle wave functions obey them. This system is solved by plane waves. Let  $k_i, n_i \in \mathbb{R}^3$ :

$$\begin{aligned}
\phi_i(x_j) &= \frac{1}{V^{\frac{1}{2}}} e^{-i\langle k_i, x_j \rangle} \\
, \text{ where } k_i &= \frac{2\pi}{L} n_i, \quad n_i = \{(n^x, n^y, n^z)^T | n^x + n^y + n^z = i\} \\
\text{and } \langle \cdot, \cdot \rangle &\text{ the canonical scalar product.}
\end{aligned} \tag{2.4}$$

The mean kinetic energy reads as:

$$\left\langle \sum_{j=i}^N \Delta_{x_i} \right\rangle = \sum_{j=i}^N \langle \Delta_{x_i} \rangle = \sum_{i=1}^N \|k_i\|^2 \tag{2.5}$$

Let the unity volume in phase space,  $B_0$ , be defined as the volume per single quantum state (in [2], this volume is equal to  $h^3$ ). With the differential element in phase space  $V dk^x dk^y dk^z$ , the differential amount of states in a spherical shell element is

$$\begin{aligned}
d\Phi &= \int_{\text{sphere}} \frac{V dk^x dk^y dk^z}{B_0} = \frac{V}{B_0} k^2 \int_0^{2\pi} \int_0^\pi \sin \vartheta_k dk d\vartheta_k d\varphi_k = \frac{4\pi V}{B_0} k^2 dk \\
, \text{ where } k &= \|k\|
\end{aligned}$$

At Fermi level, all accessible states up to the Fermi-energy are occupied, whereas no state above that level is occupied. Therefore, all occupied states form a sphere of radius  $k_F$  with the volume  $\frac{4}{3}\pi k_F^3$  in momentum space and of volume  $\frac{4}{3}\pi k_F^3 V$  in phase space. Comparing the volume in phase space with the single state volume  $B_0$ , one finds, with  $e_F = \|k_F\|^2$ , for the Fermi energy of a single state in terms of N:

$$\begin{aligned}
\frac{4}{3}\pi k_F^3 V &= B_0 N \\
e_F &= \left( \frac{3 B_0 N}{4 \pi V} \right)^{\frac{2}{3}}
\end{aligned} \tag{2.6}$$

Assuming the difference of the energy states are small, the mean kinetic energy (2.5) can be approximated at Fermi-level with

$$\begin{aligned}
\left\langle \sum_{j=i}^N \Delta_{x_i} \right\rangle &= \int_0^{k_F} k^2 d\Phi = \frac{4\pi V}{B_0} \int_0^{k_F} k^4 dk = \frac{4}{5} \frac{\pi V}{B_0} k_F^5 \\
&= \frac{3}{5} N e_F = \mathcal{O}(N^{\frac{5}{3}})
\end{aligned} \tag{2.7}$$

, where (2.6) was used. If the system is not in its ground state, the integral (2.7) has to be rewritten, using the Fermi-Dirac distribution  $f(e_F, T)$ .

$$\left\langle \sum_{j=i}^N \Delta_{x_i} \right\rangle' = \int_0^{k_{max}} f(e_f, T) k^2 d\Phi$$

But since the distribution function only relates every state to a factor, and any  $k_{max}$  can be written in terms of  $k_F$ , the dependence of the total energy on the number of particles doesn't change and the estimate (2.7) holds for  $E_F < E$ .

For estimating the interaction potential, a crucial simplification is applied: Although the particles interact with one another via the Coulomb interaction, the one particle wave functions need to be plane waves (plane waves generally don't solve entangled systems). Nevertheless, as plane waves solve the Hartree-Fock equation for a Coulomb interaction, plane waves are still sufficient for an estimate of the order in  $N$  and wave functions (2.4) can be applied to the following derivation. A justification of why solutions of the Hartree-Fock equation satisfy the assumption above is given in chapter "Argument for a time dependent Hartree-Fock equation", p. 18. In [4], it is shown, that for some wave function  $\phi$ , for as long as  $\langle E_{kin} \rangle = \mathcal{O}(N^{\frac{5}{3}})$ , the mean potential energy is bounded by  $N^2$ . This presents a more general estimate of the following than the estimate presented here.

As shown in (3.3), the mean interaction potential of the whole system for the Coulomb potential  $v_{ij}^\beta = \frac{1}{\|x_i - x_j\|_2}$  is described by:

@ {tilded

$$\begin{aligned} \left\langle \Psi, \sum_{i=1}^N \sum_{j=1}^N \frac{1}{\|x_i - x_j\|} \Psi \right\rangle &= \\ &= \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \left\langle \phi_i \phi_j, \frac{1}{\|x_1 - x_2\|} \phi_i \phi_j \right\rangle - \left\langle \phi_i \phi_j, \frac{1}{\|x_1 - x_2\|} P_{ij} \phi_i \phi_j \right\rangle \right\} \end{aligned} \quad (2.8)$$

, where the first term in the brackets is called the mean-field term and the second term is called exchange term. In the following, the interaction potential is estimated of both terms separately and  $dx_i = d^3x_i$  is the abbreviation for  $dx_i^x dx_i^y dx_i^z$ . Writing the mean-field term in integral form, it reads as:

$$\begin{aligned} &\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \int_{[0,L]^3} dx_1 \int_{[0,L]^3} dx_2 \phi_i^*(x_1) \phi_j^*(x_2) \frac{1}{\|x_1 - x_2\|} \phi_i(x_1) \phi_j(x_2) \\ &= \frac{1}{2} \sum_{j=1}^N \int_{[0,L]^3} dx_2 \phi_j^*(x_2) \int_{[0,L]^3} dx_1 \frac{1}{\|x_1 - x_2\|} \sum_{i=1}^N |\phi_i(x_1)|^2 \phi_j(x_2) \end{aligned}$$

As  $\phi_i(x_j) = \frac{1}{V^{\frac{1}{2}}} e^{-i\langle k_i, x_j \rangle}$ ,  $\|\phi_i\|^2 = \frac{1}{V}$ , the expression above simplifies to:

$$\begin{aligned}
& \frac{N}{2V} \int_{[0,L]^3} dx_2 \sum_{j=1}^N \|\phi_j(x_2)\|^2 \int_{[0,L]^3} dx_1 \frac{1}{\|x_1 - x_2\|} \\
&= \frac{N^2}{2V^2} \int_{[0,L]^3} dx_2 \int_{[0,L]^3} dx_1 \frac{1}{\|x_1 - x_2\|}
\end{aligned}$$

Because the integrals are finite, it is clear, that this term is of order  $\mathcal{O}(N^2)$ .

Now, writing the exchange term in (2.8) in integral form and inserting plane wave functions (2.4) leads to:

$$\begin{aligned}
& \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \left\langle \phi_i \phi_j, \frac{1}{\|x_1 - x_2\|} P_{ij} \phi_i \phi_j \right\rangle \right\} \\
&= \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \int_{[0,L]^3} dx_1 \int_{[0,L]^3} dx_2 \phi_i^*(x_1) \phi_j^*(x_2) \frac{1}{\|x_1 - x_2\|} \phi_i(x_2) \phi_j(x_1) \\
&= \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \int_{[0,L]^3} dx_1 \int_{[0,L]^3} dx_2 \frac{1}{V^2} e^{i\langle k_i, x_1 - x_2 \rangle} e^{-i\langle k_j, x_1 - x_2 \rangle} \frac{1}{\|x_1 - x_2\|} \\
&= \frac{1}{2V^2} \sum_{i=1}^N \sum_{j=1}^N \int_{[0,L]^3} dx_1 \int_{[0,L]^3} dx_2 e^{i\langle k_i - k_j, x_1 - x_2 \rangle} \frac{1}{\|x_1 - x_2\|} \\
&= \frac{1}{2V^2} \sum_{i=1}^N \sum_{j=1}^N \int_{[0,L]^3} dx_1 \int_{[0,L]^3 + x_1} dx' e^{i\langle k_i - k_j, x' \rangle} \frac{1}{\|x'\|} \\
&\lesssim \frac{1}{2V^2} \sum_{i=1}^N \sum_{j=1}^N \int_{[0,L]^3} dx_1 \int_{\mathbb{R}^3} dx' e^{i\langle k_i - k_j, x' \rangle} \frac{1}{\|x'\|}
\end{aligned}$$

, where, in the second last step, the relative coordinate  $x' = x_1 - x_2$ ,  $dx' = dx_1$  was defined. In auxiliary calculation "Fourier transformation of Coulomb potential", p. 29, it is shown, that the last integral is the Fourier transformation of  $\frac{4\pi}{\|k_i - k_j\|^2}$ . Using this relation, the term above now reads as:

$$\frac{2\pi}{V^2} \sum_{i=1}^N \sum_{j=1}^N \int_{[0,L]^3} dx_1 \frac{1}{\|k_i - k_j\|^2} = \frac{2\pi}{V} \sum_{i=1}^N \sum_{j=1}^N \frac{1}{\|k_i - k_j\|^2} \quad (2.9)$$

Again, the system is assumed to be in its ground state and the difference between the k-states is assumed to be small. The sums above can therefore be approximated by integrals over spheres with the Fermi radius  $k_F$ . Furthermore, approximating the term above for  $k_i = 0$ , the integration is symmetric around 0 and therefore gives its biggest contribution.

$$\begin{aligned}
& \frac{2\pi}{V} \int_{B_{k_F}} dk_i \int_{B_{k_F}} dk_j \frac{1}{\|k_i - k_j\|^2} \leq \frac{2\pi}{V} \int_{B_{k_F}} dk_i \int_{B_{k_F}} dk_j \frac{1}{\|k_j\|^2} \\
&= \frac{8\pi^2}{V} k_F \int_{B_{k_F}} dk_i = \frac{32\pi^3}{3V} k_F^4 \sim N^{\frac{4}{3}}
\end{aligned}$$

As the mean- field term is of order  $\mathcal{O}(N^2)$  and the exchange term only of order  $\mathcal{O}(N^{\frac{4}{3}})$  in  $N$ , the whole interaction term is of order  $\mathcal{O}(N^2)$ . The exchange term is therefore negligible in the mean- field limit  $N \rightarrow \infty$ . With the estimates of the kinetic energy  $\mathcal{O}(N^{\frac{5}{3}})$  and the interaction potential  $\mathcal{O}(N^2)$ , the parameters  $a, b$  in (2.3) can be determined such that the scaled kinetic energy and interaction potential are of same order in  $N$ :

$$2b - a + \frac{5}{3} = b - a + 2$$

Suggesting that both, kinetic energy and interaction potential, should be of order  $\mathcal{O}(N)$ , this equation is solved for  $a = \frac{4}{3}$  and  $b = \frac{1}{3}$ . Applying  $a, b$  to (2.3), the Hamiltonian for this system reads as:

$$i\partial_t\Psi(\underline{x}, t) = -N^{-\frac{2}{3}}\sum_{i=1}^N\Delta_{x_i}\Psi(\underline{x}, t) + N^{-1}\sum_{1\leq i<j\leq N}\frac{1}{\|x_i - x_j\|}\Psi(\underline{x}, t)$$

But with this scaling arises another problem, when it is applied to estimate mean-field limits: As the kinetic energy per particle is of order  $\mathcal{O}(N^{\frac{2}{3}})$ , the particles velocity is of order  $\mathcal{O}(N^{\frac{1}{3}})$ . Observing the system for some time of order one,  $\mathcal{O}(N^{\frac{1}{3}})$  interactions occur and in the mean-field limit  $N \rightarrow \infty$ , no proposition about a mean-field approximation can be made: It is not possible to compare a slightly time-developed initial state in a mean-field with a slightly time-developed wave function that starts to entangle for that many interactions. This problem is comparable to the attempt of analysing a mean-field behaviour for infinite times. A solution to this problem is obtained when  $\partial_t \rightarrow N^{-\frac{1}{3}}\partial_t$  is applied to the Hamiltonian. Using this argument, the Hamiltonian above therefore becomes:

$$iN^{-\frac{1}{3}}\partial_t\Psi(\underline{x}, t) = -N^{-\frac{2}{3}}\sum_{i=1}^N\Delta_{x_i}\Psi(\underline{x}, t) + N^{-1}\sum_{1\leq i<j\leq N}\frac{1}{\|x_i - x_j\|}\Psi(\underline{x}, t)$$

Note that kinetic energy and interaction potential are still of the same order.

The applicability of a mean-field approximation of this system has been investigated, among other publications, in [1] and [3]. The paper [1] proofs, that there exists a  $T$ , such that for all  $t < T$ , the one particle density matrix  $\gamma_{N,t}^{(1)}$ , which describes the time evolution of the system, converges towards a one particle density matrix  $\omega_{N,t}$ , which is the solution of the Hartree equation:

$$i\hbar\partial_t\omega_{N,t} = [-\hbar^2\Delta + (V * \rho_t), \omega_{N,t}]$$

In [3], this result is developed further for arbitrary times of order one and less restrictions on the interaction potential.

## 2.3 Volume linear in $N$

In this chapter, a system is considered, of which the volume is proportional to the number of particles. Again, a box of volume  $V = V(N) = V_0N = L_0^3N$

is successively filled with fermions, but as the box is filled, its volume increases proportionally to the number of particles.

The estimate for the kinetic and potential energy are very similar to the case of the box with fixed volume and therefore, the derivations refer to the other case often.

The one particle wave function changes in its normalization factor and its momentum:

$$\phi_i(x_j) = \frac{1}{V_0^{\frac{1}{2}} N^{\frac{1}{2}}} e^{-i\langle k_i, x_j \rangle} \quad (2.10)$$

, where  $k_i = \frac{2\pi n_i}{L_0 N^{\frac{1}{3}}}$ .

As  $V$  is a function of  $N$  now, the differential amount of states in a spherical shell element in phase space now reads as:

$$\begin{aligned} d\Phi &= \int_{\text{sphere}} \frac{V dN dk^x dk^y dk^z}{B_0} = \frac{V}{B_0} k^2 \int_0^{2\pi} \int_0^\pi \sin \vartheta_k dk d\vartheta_k d\varphi_k dN \\ &= \frac{4\pi V}{B_0} k^2 dk dN \end{aligned}$$

The sphere of states at Fermi-level in phase space now becomes  $\frac{4}{3}\pi k_F^3 V(N)$  and with  $V(N) = V_0 N$ , equation (2.6) changes to:

$$\begin{aligned} \frac{4}{3}\pi k_F^3 N V_0 &= B_0 N \\ e_F &= \left( \frac{3 B_0}{4 \pi V_0} \right)^{\frac{2}{3}} \end{aligned} \quad (2.11)$$

for some unitary volume  $V_0$  in coordinate space. It is important to notice, that the energy of a single particle at Fermi level (2.11) does not depend on  $N$  any more. Using the differential amount of states in a spherical shell element and approximating the sum over all one-particle energies by an integral, the mean kinetic energy is:

$$\begin{aligned} \left\langle \sum_{j=i}^N \Delta_{x_i} \right\rangle &= \int_0^{k_F} k^2 d\Phi = \frac{4\pi V_0}{B_0} \int_0^N \int_0^{k_F} k^4 dk dN = \frac{4}{5} \frac{\pi V_0}{B_0} k_F^5 N \\ &= \frac{3}{5} e_F N = \mathcal{O}(N) \end{aligned}$$

This is directly proportional to the number of particles  $N$  and doesn't depend on  $V_0$ . Using the same argument from the first derivation, the estimate holds for mean kinetic energies bigger than the Fermi-energy  $E_F$ .

In the same manner as in the case of a box of constant volume, the one-particle wave functions are assumed to be plane wave functions, as defined in (2.10).

$$\begin{aligned}
& \left\langle \Psi, \sum_{i=1}^N \sum_{j=1}^N \frac{1}{\|x_i - x_j\|} \Psi \right\rangle \\
&= \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \left\langle \phi_i \phi_j, \frac{1}{\|x_1 - x_2\|} \phi_i \phi_j \right\rangle - \left\langle \phi_i \phi_j, \frac{1}{\|x_1 - x_2\|} P_{ij} \phi_i \phi_j \right\rangle \right\}
\end{aligned} \tag{2.12}$$

Again, the estimates of the order on  $N$  of the terms above is done for the mean-field term and the exchange term separately. The mean-field term in integral form reads as:

$$\begin{aligned}
& \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \left\langle \phi_i \phi_j, \frac{1}{\|x_1 - x_2\|} \phi_i \phi_j \right\rangle \right\} \\
&= \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \int_{[0,L]^3} \int_{[0,L]^3} dx_1 dx_2 \phi_i^*(x_1) \phi_j^*(x_2) \frac{1}{\|x_1 - x_2\|} \phi_i(x_1) \phi_j(x_2) \\
&= \frac{1}{2} \sum_{j=1}^N \int_{[0,L]^3} dx_2 \phi_j^*(x_2) \int_{[0,L]^3} dx_1 \frac{1}{\|x_1 - x_2\|} \sum_{i=1}^N \|\phi_i(x_1)\|^2 \phi_j(x_2)
\end{aligned}$$

In auxiliary calculation "order in  $N$  of the convolution", p. 29, it is shown, that the convolution in the term above is of order  $\mathcal{O}(N^{\frac{2}{3}})$ . Note, that the density of states  $\sum_{i=1}^N |\phi_i|^2 = \frac{N}{V} = \frac{1}{V_0}$  is independent of  $N$ . Applying this to the term above leads to:

$$\leq \frac{1}{2} \sum_{j=1}^N \int_{[0,L]^3} dx_2 \phi_j^*(x_2) \frac{2\pi}{V_0^{\frac{1}{3}}} N^{\frac{2}{3}} \phi_j(x_2) = \frac{1}{V_0} V_0 N \frac{\pi}{V_0^{\frac{1}{3}}} N^{\frac{2}{3}} = \frac{\pi}{V_0^{\frac{1}{3}}} N^{\frac{5}{3}}$$

The mean-field term is therefore of order  $\mathcal{O}(N^{\frac{5}{3}})$ . In the following, the order of the exchange term of (2.12) is estimated:

$$\begin{aligned}
& \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \left\langle \phi_i \phi_j, \frac{1}{\|x_1 - x_2\|} P_{ij} \phi_i \phi_j \right\rangle \right\} \\
& \lesssim \frac{1}{2V_0^2 N^2} \sum_{i=1}^N \sum_{j=1}^N \int_{[0, L_0 N^{\frac{1}{3}}]^3} dx_1 \int_{\mathbb{R}^3} dx' e^{i(k_i - k_j, x')} \frac{1}{\|x'\|} \\
& = \frac{2\pi}{V_0^2 N^2} \sum_{i=1}^N \sum_{j=1}^N \int_{[0, L_0 N^{\frac{1}{3}}]^3} dx_1 \frac{1}{\|k_i - k_j\|^2} \\
& = \frac{2\pi}{V_0 N} \sum_{i=1}^N \int_{B_{k_F}} dk_j V_0 N \frac{1}{\|k_i - k_j\|^2} \\
& \approx 2\pi V_0 N \int_{B_{k_F}} dk_i \int_{B_{k_F}} dk_j \frac{1}{\|k_i - k_j\|^2} \\
& \leq 2\pi V_0 N \int_{B_{k_F}} dk_i \int_{B_{k_F}} dk_j \frac{1}{\|k_j\|^2} \\
& = 8\pi^2 V_0 N k_F \int_{B_{k_F}} dk_i = \frac{32\pi^3 k_F^4}{3} V_0 N
\end{aligned}$$

As seen in the calculation above, the kinetic energy is of order  $\mathcal{O}(N)$ , the mean-field term is of order  $\mathcal{O}(N^{\frac{5}{3}})$  and the exchange term is of order  $\mathcal{O}(N)$ . Like in the first case, for a constant volume, the exchange term is of smaller order than the mean-field term and therefore, can be neglected for the mean-field limit  $N \rightarrow \infty$ . The whole interaction term, the sum of the mean-field term and exchange term, is of order  $\mathcal{O}(N^{\frac{5}{3}})$ . Applying this to (2.3), this leads to the condition of the kinetic term and the interaction term to be of the same order in  $N$  for the scaled Hamiltonian:

$$2b - a + 2 = b - a + \frac{5}{3}$$

If the two scaled terms should be of order  $\mathcal{O}(N)$ , the parameters  $a = \frac{4}{3}$  and  $\frac{2}{3}$  solve the equation above and the scaled Hamiltonian (2.3) reads as:

$$\begin{aligned}
H &= - \sum_{i=1}^N \Delta_{x_j} + N^{-\frac{2}{3}} \sum_{1 \leq i < j \leq N} \frac{1}{\|x_i - x_j\|} \\
i\partial_t \Psi(x, t) &= H \Psi(x, t)
\end{aligned} \tag{2.13}$$

The kinetic energy per particle is constant and therefore, the problem with the observability of the system, which arises for the system with constant volume, doesn't arise in this system.





### 3 Derivation of the Hartree-Fock equations for fermionic systems

Assume, a many-particle system of fermions in an external potential  $A^t$  (for example an attractive Coulomb potential representing a nucleus). Each of the  $N$  particles does not only interact with  $A^t$ , but also with the other  $N - 1$  particles via the Coulomb interaction. The Hartree-Fock equations approximate for every particle the many particle interaction with a mean-interaction generated by all other particles, whose  $N$  particles interact only with  $A^t$  and a background potential which is generated by the  $N - 1$  other particles, respectively. These equations, therefore, form a (stationary) mean-field of the fermionic system.

In the following, the Hartree-Fock equations are derived with the variation method, i.e. by minimizing the total energy of the system. It is due to this method, that the equations are stationary. But as in the following chapter, "An approach to a mean-field approximation", p. 21, the dynamics of an initially approximable system is investigated, in the end of this chapter, an argument for a dynamic Hartree-Fock equation, on the grounds of the stationary Hartree-Fock equation, is given.

This derivation is included to this thesis, as it explains the appearance of two very interesting features. Firstly, it explains the appearance of the exchange term which is due to the nature of fermions, entirely. And secondly, because it shows, that the equations are not linear.

#### 3.1 The stationary Hartree-Fock equations

Assuming a system of interacting fermions with an external potential, the Hamiltonian reads as:

$$H = - \sum_{n=1}^N \alpha \Delta_{x_n} + A^t(x_n) + \sum_{1 \leq i < j \leq N} v_{ij}^\beta = H_1 + H_2$$

$$, \text{ where } H_1 = \sum_{i=1}^N h^{(i)} = - \sum_{n=1}^N \alpha \Delta_{x_n} + A^t(x_n) \quad \text{and} \quad H_2 = \sum_{1 \leq i < j \leq N} v_{ij}^\beta$$

$$i\partial_t \Psi = H\Psi$$

$H_1$  describes the kinetic term, with some scaling parameter  $\alpha$ , and the interaction with an external potential  $A^t$  whereas  $H_2$  describes the pairwise interaction of particles at coordinates  $x_i$  and  $x_j$ .  $H_2$  is called the interaction Hamiltonian, it consists of  $\binom{N}{2} = \frac{1}{2}N(N-1)$  terms. The potential  $v_{ij}^\beta$  is of the form  $N^\beta V_N(x_i - x_j)$ ,

where  $\beta$  is a scaling parameter, and supposed to be symmetric with respect to particle exchange:  $v_{ij}^\beta = v_{ji}^\beta$ . This potential could, for example, describe a Coulomb potential, like in chapter "Scalings". In the following, this Hamiltonian is applied to a fermion state, i.e. a Slater determinant of the form defined in (1.1):

$$\Psi(\underline{x}) = \left( \bigwedge_{j=1}^N \phi_j \right) (\underline{x}) = \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_n} \text{sgn}(\sigma) \prod_{j=1}^N \phi_j(x_{\sigma_j}) = \sqrt{N!} A \prod_{j=1}^N \phi_j(x_{\sigma_j})$$

, where  $A = \frac{1}{N!} \sum_{\sigma \in S_n} \text{sgn}(\sigma)$  is the antisymmetrization projector.

It is important to notice, that the sum over the permutations solely acts on the the coordinates  $x_{\sigma_j}$ , whereas the product acts on the states  $\phi_j$ . Keeping that in mind, the coordinates are not explicitly stated in the scalar products following.

The expectation value of  $H$  is equal to the sum of  $H_1$  and  $H_2$ :

$$\langle \Psi, H\Psi \rangle = \langle \Psi, H_1\Psi \rangle + \langle \Psi, H_2\Psi \rangle \quad (3.1)$$

$$\begin{aligned} \langle \Psi, H_1\Psi \rangle &= \left\langle \Psi, \sum_{i=1}^N h^{(i)}\Psi \right\rangle \\ &= \sum_{i=1}^N \left\langle \sqrt{N!}A \prod_{l=1}^N \phi_l, h^{(i)} \sqrt{N!}A \prod_{k=1}^N \phi_k \right\rangle \\ &= N! \sum_{i=1}^N \left\langle \prod_{l=1}^N \phi_l, h^{(i)} A^2 \prod_{k=1}^N \phi_k \right\rangle \\ &= N! \sum_{i=1}^N \left\langle \prod_{l=1}^N \phi_l, h^{(i)} A \prod_{k=1}^N \phi_k \right\rangle \\ &= N! \sum_{i=1}^N \left\langle \prod_{l=1}^N \phi_l, h^{(i)} \frac{1}{N!} \sum_{\sigma \in S_n} \text{sgn}(\sigma) \prod_{k=1}^N \phi_k \right\rangle \\ &= \sum_{i=1}^N \left\langle \prod_{l=1}^N \phi_l, h^{(i)} \prod_{k=1}^N \phi_k \right\rangle = \sum_{i=1}^N \langle \phi_i, h^{(i)} \phi_i \rangle \end{aligned} \quad (3.2)$$

The one particle wave functions form an orthonormal system and therefore, the scalar product is equal is zero for every permutation, except for the one term, whose states are not exchanged. This was taken advantage of in the second last step.

$$\begin{aligned}
\langle \Psi, H_2 \Psi \rangle &= \left\langle \sqrt{N!} A \prod_{l=1}^N \phi_l, \sum_{1 \leq i < j \leq N} v_{ij}^\beta \sqrt{N!} A \prod_{k=1}^N \phi_k \right\rangle \\
&= N! \sum_{1 \leq i < j \leq N} \left\langle \prod_{l=1}^N \phi_l, v_{ij}^\beta A \prod_{k=1}^N \phi_k \right\rangle \\
&= \sum_{1 \leq i < j \leq N} \left\{ \left\langle \prod_{l=1}^N \phi_l, v_{ij}^\beta \prod_{k=1}^N \phi_k \right\rangle - \left\langle \prod_{l=1}^N \phi_l, v_{ij}^\beta P_{ij} \prod_{k=1}^N \phi_k \right\rangle \right\} \quad (3.3) \\
&= \sum_{1 \leq i < j \leq N} \left\{ \left\langle \phi_i \phi_j, v_{ij}^\beta \phi_i \phi_j \right\rangle - \left\langle \phi_i \phi_j, v_{ij}^\beta P_{ij} \phi_i \phi_j \right\rangle \right\} \\
&= \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \left\langle \phi_i \phi_j, v_{ij}^\beta \phi_i \phi_j \right\rangle - \left\langle \phi_i \phi_j, v_{ij}^\beta P_{ij} \phi_i \phi_j \right\rangle \right\} \\
&= \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \left\langle \phi_i \phi_j, v_{12}^\beta \phi_i \phi_j \right\rangle - \left\langle \phi_i \phi_j, v_{12}^\beta P_{ij} \phi_i \phi_j \right\rangle \right\}
\end{aligned}$$

As from here on, the only coordinates of interest are those of  $\phi_i$  and  $\phi_j$ ; they are renamed to  $x_1$  and  $x_2$  for simplicity. The interaction potential now acts on  $x_1$  and  $x_2$ :  $v_{ij}^\beta \rightarrow v_{12}^\beta$ . In the term above, the first term in the brackets is called mean-field term, which describes the pairwise interaction of  $\phi_i$  and  $\phi_j$ . The second term is called exchange term. It describes the potential due to the transposition of two one- particle states in space. This is a purely quantum mechanical effect, that arises exclusively from the nature of the fermions.

For a stationary state, the energy is assumed to minimize. In the following, a one- particle wave function is looked for which minimizes (3.1) This procedure is called the variation method and its earlier mentioned problem with time dependent systems is commented on in the end of this chapter.

As well as this requirement, the derived N-particle wave function (consisting of one particle solutions of the minimization problem) must still be written as a Slater determinant, e.g. the one particle solutions must be an orthonormal system. Using that, the constraint to the variation is:

$$\langle \phi_i, \phi_j \rangle - \delta_{ij} = 0$$

and therefore, the variation problem reads as:

$$L = \langle \Psi, H \Psi \rangle - \left[ \sum_{i=1}^N \sum_{j=1}^N e_{ij} (\langle \phi_i, \phi_j \rangle - \delta_{ij}) \right]$$

, where  $e_{ij}$  are Lagrange multipliers. In auxiliary calculation "Lagrange multipliers  $e_{ij}$  are diagonalizable", p. 29, it is shown that  $e_{ij}$  is diagonalizable, what leads to the equivalent but simpler equation:

$$\begin{aligned}
L &= \langle \Psi, H\Psi \rangle - \left[ \sum_{i=1}^N e_{ii} (\langle \phi_i, \phi_i \rangle - 1) \right] \\
&= \sum_{i=1}^N \langle \phi_i, h^{(i)} \phi_i \rangle + \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle \phi_i \phi_j, v_{12}^\beta \phi_i \phi_j \rangle - \langle \phi_i \phi_j, v_{12}^\beta P_{ij} \phi_i \phi_j \rangle \right\} \quad (3.4) \\
&\quad - \sum_{i=1}^N e_{ii} (\langle \phi_i, \phi_i \rangle - 1)
\end{aligned}$$

Applying the variation condition  $\phi \longrightarrow \phi + \delta\phi$  leads to:

$$\begin{aligned}
\delta L &= \sum_{i=1}^N \left\{ \langle \delta\phi_i, h^{(i)} \phi_i \rangle + \langle \phi_i, h^{(i)} \delta\phi_i \rangle \right\} \\
&\quad + \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle \delta\phi_i \phi_j, v_{12}^\beta \phi_i \phi_j \rangle + \langle \phi_i \delta\phi_j, v_{12}^\beta \phi_i \phi_j \rangle \right. \\
&\quad \left. + \langle \phi_i \phi_j, v_{12}^\beta \delta\phi_i \phi_j \rangle + \langle \phi_i \phi_j, v_{12}^\beta \phi_i \delta\phi_j \rangle \right\} \\
&\quad - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle \delta\phi_i \phi_j, v_{12}^\beta P_{ij} \phi_i \phi_j \rangle + \langle \phi_i \delta\phi_j, v_{12}^\beta P_{ij} \phi_i \phi_j \rangle \right. \\
&\quad \left. + \langle \phi_i \phi_j, v_{12}^\beta P_{ij} \delta\phi_i \phi_j \rangle + \langle \phi_i \phi_j, v_{12}^\beta P_{ij} \phi_i \delta\phi_j \rangle \right\} \\
&\quad - \sum_{i=1}^N \{ \langle \delta\phi_i, \phi_i \rangle + \langle \phi_i, \delta\phi_i \rangle \} = 0
\end{aligned}$$

The two terms in the first line are the complex conjugated of one another. That is the same case for the two terms in the last line. The other terms have a complex conjugated partner term as well. Using the following identity,

$$\begin{aligned}
\langle \delta\phi_i \phi_j, v_{12}^\beta \phi_i \phi_j \rangle &= \int \int dx_1 dx_2 \delta\phi_i^*(x_1) \phi_j^*(x_2) v_{12}^\beta \phi_i(x_1) \phi_j(x_2) \\
&= \int \int dx_2 dx_1 \phi_j^*(x_2) \delta\phi_i^*(x_1) v_{12}^\beta \phi_j(x_2) \phi_i(x_1) = \langle \phi_j \delta\phi_i, v_{12}^\beta \phi_j \phi_i \rangle
\end{aligned}$$

it is obvious, that the first term in the second line is the complex conjugated of the first term in the third line. With an analogous calculation, the other complex conjugated terms are discovered. Using this, the variation equation simplifies further to:

$$\begin{aligned}
\delta L &= \sum_{i=1}^N \langle \delta \phi_i, h^{(i)} \phi_i \rangle \\
&+ \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle \delta \phi_i \phi_j, v_{12}^\beta \phi_i \phi_j \rangle + \langle \delta \phi_j \phi_i, v_{12}^\beta \phi_j \phi_i \rangle \right\} \\
&- \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle \delta \phi_i \phi_j, v_{12}^\beta P_{ij} \phi_i \phi_j \rangle + \langle \delta \phi_j \phi_i, v_{12}^\beta P_{ij} \phi_j \phi_i \rangle \right\} \\
&- \sum_{i=1}^N e_i \langle \delta \phi_i, \phi_i \rangle + c.c. = 0
\end{aligned}$$

Here and in the following, *c.c.* denotes the complex conjugated of the whole term before.

Both double sums run over all possible combinations of particle states. Therefore, every combination is counted twice and  $\delta L$  can be shortened to:

$$\begin{aligned}
\delta L &= \sum_{i=1}^N \langle \delta \phi_i, h^{(i)} \phi_i \rangle \\
&+ \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle \delta \phi_i \phi_j, v_{12}^\beta \phi_i \phi_j \rangle - \langle \delta \phi_i \phi_j, v_{12}^\beta P_{ij} \phi_i \phi_j \rangle \right\} \\
&- \sum_{i=1}^N e_i \langle \delta \phi_i, \phi_i \rangle + c.c. \\
&= \sum_{i=1}^N \int dx_1 \delta \phi_i^*(x_1) \\
&* \left[ h^{(i)} \phi_i + \sum_{j=1}^N \int dx_2 \phi_j^*(x_2) v_{12}^\beta \phi_i(x_1) \phi_j(x_2) \right. \\
&\quad \left. - \sum_{j=1}^N \int dx_2 \phi_j^*(x_2) v_{12}^\beta P_{ij} \phi_i(x_1) \phi_j(x_2) - e_i \phi_i \right] + c.c. \\
&= \sum_{i=1}^N \int dx_1 \delta \phi_i^*(x_1) \\
&* \left[ h^{(i)} + \sum_{j=1}^N \int dx_2 v_{12}^\beta |\phi_j(x_2)|^2 - \sum_{j=1}^N \int dx_2 \phi_j^*(x_2) v_{12}^\beta P_{ij} \phi_j(x_1) - e_i \right] * \phi_i(x_1) \\
&+ c.c. = 0
\end{aligned}$$

In auxiliary calculation "Simplifying the complex conjugated term of the variation equation" ,p 30, it is demonstrated, that from the complex conjugated term in the expression above evolves the same term as in the square brackets above.

Therefore, this variation equation is satisfied if, the term in the square brackets is equal to zero. Inserting the definitions of  $h^{(i)}$  and  $v_{12}^\beta$  and reintroducing, that  $x_1 = x_i$  and  $x_2 = x_j$ , the coordinates of  $\phi_i$  and  $\phi_j$ , respectively, leads to:

$$\begin{aligned}
0 &= -\Delta_{x_i} + A^t(x_i) + \sum_{j=1}^N \int dx_j N^\beta V_N(x_i - x_j) |\phi_j(x_j)|^2 \\
&\quad - \sum_{j=1}^N \int dx_j \phi_j^*(x_j) N^\beta V_N(x_i - x_j) P_{ij} \phi_j(x_j) - e_i \\
e_i &= -\Delta_{x_i} + A^t(x_i) + N^\beta \left( V_N * \sum_{j=1}^N |\phi_j|^2 \right) (x_i) \\
&\quad - N^\beta \sum_{j=1}^N \int dx_j \phi_j^*(x_j) V_N(x_i - x_j) P_{ij} \phi_j(x_j)
\end{aligned} \tag{3.5}$$

This is the Hartree- Fock equation for fermions systems. The Lagrange multipliers are interpreted as energies of the one particle wave function. Note, that it depends on the particle density  $\sum_{j=1}^N |\phi_j|^2$  itself and is therefore not linear! Neglecting the second line in (3.5), the exchange term, the equation is called the Hartree equation. There are cases in which it is justified to neglect the exchange term, as for example in the two described systems in chapter "Scalings".

Solutions  $\phi$  of the derived equation minimize the total energy of a system. And therefore, a Slater determinant, consisting of these  $\phi$  describes a ground state of a fermion system.

### 3.2 Argument for a time dependent Hartree-Fock equation

This chapter gives an argument for why one particle wave functions, that satisfy (3.5), should also satisfy a time dependent Hartree-Fock equation of the form:

$$\begin{aligned}
h_i^{HF} &= -\Delta_{x_i} + A^t(x_i) + N^\beta \left( V_N * \sum_{j=1}^N |\phi_j|^2 \right) (x_i) \\
&\quad - N^\beta \sum_{j=1}^N \int dx_j \phi_j^*(x_j) V_N(x_i - x_j) P_{ij} \phi_j(x_j) \\
\text{with } i\partial_t \phi^t &= h_i^{HF} \phi^t
\end{aligned} \tag{3.6}$$

As the energy of a system is assumed to be constant, the time derivative of the variation functional (3.4) is zero. If this derivative is shown to be zero with solutions of (3.6), these one particle wave function keep the total energy of the system constant. This is a necessary requirement of the validity of (3.6).

Solutions of the stationary Hartree-Fock equation (3.5) minimize the energy for some time  $t = 0$ . If for  $t = 0$ , the  $N$ -particle wave function  $\Psi$  can be written as a Slater determinant of solutions of the stationary Hartree-Fock equation (3.5), the total energy of the system is  $E \left( \bigwedge_{j=1}^N \phi_j^0 \right) = E(\Psi^0)$ . The time derivative of (3.4) reads as:

$$\begin{aligned}
\partial_t L &= \partial_t \left\{ \sum_{i=1}^N \langle \phi_i, h^{(i)} \phi_i \rangle + \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle \phi_i \phi_j, v_{12}^\beta \phi_i \phi_j \rangle - \langle \phi_i \phi_j, v_{12}^\beta P_{ij} \phi_i \phi_j \rangle \right\} \right. \\
&\quad \left. - \sum_{i=1}^N e_{ii} (\langle \phi_i, \phi_i \rangle - 1) \right\} \\
&= \sum_{i=1}^N \left\{ \langle \partial_t \phi_i, h^{(i)} \phi_i \rangle + \langle \phi_i, h^{(i)} \partial_t \phi_i \rangle \right\} \\
&\quad + \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle (\partial_t \phi_i) \phi_j, v_{12}^\beta \phi_i \phi_j \rangle + \langle \phi_i (\partial_t \phi_j), v_{12}^\beta \phi_i \phi_j \rangle \right. \\
&\quad \quad \left. + \langle \phi_i \phi_j, v_{12}^\beta (\partial_t \phi_i) \phi_j \rangle + \langle \phi_i \phi_j, v_{12}^\beta \phi_i (\partial_t \phi_j) \rangle \right\} \\
&\quad - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle (\partial_t \phi_i) \phi_j, v_{12}^\beta P_{ij} \phi_i \phi_j \rangle + \langle \phi_i (\partial_t \phi_j), v_{12}^\beta P_{ij} \phi_i \phi_j \rangle \right. \\
&\quad \quad \left. + \langle \phi_i \phi_j, v_{12}^\beta P_{ij} (\partial_t \phi_i) \phi_j \rangle + \langle \phi_i \phi_j, v_{12}^\beta P_{ij} \phi_i (\partial_t \phi_j) \rangle \right\} \\
&\quad - \sum_{i=1}^N e_{ii} \{ \langle \partial_t \phi_i, \phi_i \rangle + \langle \phi_i, \partial_t \phi_i \rangle \} \\
&= i \sum_{i=1}^N \left\{ \langle h_i^{HF} \phi_i, h^{(i)} \phi_i \rangle - \langle \phi_i, h^{(i)} h_i^{HF} \phi_i \rangle \right\} \\
&\quad + i \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle h_1^{HF} \phi_i \phi_j, v_{12}^\beta \phi_i \phi_j \rangle + \langle h_2^{HF} \phi_i \phi_j, v_{12}^\beta \phi_i \phi_j \rangle \right. \\
&\quad \quad \left. - \langle \phi_i \phi_j, v_{12}^\beta h_1^{HF} \phi_i \phi_j \rangle - \langle \phi_i \phi_j, v_{12}^\beta h_2^{HF} \phi_i \phi_j \rangle \right\} \\
&\quad - i \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle h_1^{HF} \phi_i \phi_j, v_{12}^\beta P_{ij} \phi_i \phi_j \rangle + \langle h_2^{HF} \phi_i \phi_j, v_{12}^\beta P_{ij} \phi_i \phi_j \rangle \right. \\
&\quad \quad \left. - \langle \phi_i \phi_j, v_{12}^\beta P_{ij} h_1^{HF} \phi_i \phi_j \rangle - \langle \phi_i \phi_j, v_{12}^\beta P_{ij} h_2^{HF} \phi_i \phi_j \rangle \right\} \\
&\quad - i \sum_{i=1}^N e_{ii} \{ \langle h_1^{HF} \phi_i, \phi_i \rangle - \langle \phi_i, h_2^{HF} \phi_i \rangle \}
\end{aligned}$$

$$\begin{aligned}
&= i \sum_{i=1}^N \langle \phi_i, [h_1^{HF}, h^{(1)}] \phi_i \rangle \\
&\quad + i \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle \phi_i \phi_j, [h_1^{HF}, v_{12}^\beta] \phi_i \phi_j \rangle + \langle \phi_i \phi_j, [h_2^{HF}, v_{12}^\beta] \phi_i \phi_j \rangle \right\} \\
&\quad - i \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle \phi_i \phi_j, [h_1^{HF}, v_{12}^\beta P_{ij}] \phi_i \phi_j \rangle + \langle \phi_i \phi_j, [h_2^{HF}, v_{12}^\beta P_{ij}] \phi_i \phi_j \rangle \right\}
\end{aligned}$$

Applying the definitions to the commutators, it is possible to simplify them:

$$\begin{aligned}
h^{(i)} &= -\Delta_{x_i} + A^t(x_i) \\
v_{12}^\beta &= N^\beta V_N(x_1 - x_2) \\
v_{mf} &= N^\beta \left( V_N * \sum_{j=1}^N |\phi_j|^2 \right) (x_i) - N^\beta \sum_{j=1}^N \int dx_j \phi_j^*(x_j) V_N(x_i - x_j) P_{ij} \phi_j(x_j) \\
[h_1^{HF}, h^{(1)}] &= [v_{mf}(x_1), h^{(1)}] \\
[h_1^{HF}, v_{12}^\beta] &= [h^{(1)}, v_{12}^\beta] + [v_{mf}(x_1), v_{12}^\beta] = [h^{(1)}, v_{12}^\beta]
\end{aligned}$$

Applying these commutators to the terms above leads to:

$$\begin{aligned}
&= -i \sum_{i=1}^N \langle \phi_i, [h^{(1)}, v_{mf}(x_1)] \phi_i \rangle \\
&\quad + i \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle \phi_i \phi_j, [h^{(1)}, v_{12}^\beta] \phi_i \phi_j \rangle - \langle \phi_i \phi_j, [h^{(1)}, v_{12}^\beta P_{ij}] \phi_i \phi_j \rangle \right\} \\
&= 2 \sum_{i=1}^N \text{Im} \left\{ \langle \phi_i, h^{(1)} v_{mf}(x_1) \phi_i \rangle \right. \\
&\quad \left. - \left( \sum_{j=1}^N \langle \phi_i \phi_j, h^{(1)} v_{12}^\beta \phi_i \phi_j \rangle - \sum_{j=1}^N \langle \phi_i \phi_j, h^{(1)} v_{12}^\beta P_{ij} \phi_i \phi_j \rangle \right) \right\} \\
&= 0
\end{aligned}$$

Therefore, one particle wave functions  $\phi$  that satisfy (3.6) conserve the total energy for some time  $t$ :

$$E \left( \bigwedge_{j=1}^N \phi_j^t \right) = E \left( \bigwedge_{j=1}^N \phi_j^0 \right) = E(\Psi^0) = E(\Psi^t)$$

As mentioned above, this is only a motivation for why wave functions  $\phi$ , satisfy the stationary Hartree-Fock equation (3.5), also satisfy the time dependent Hartree-Fock equation (3.6).



## 4 An approach to a mean-field approximation

This chapter aims to introduce a method of how to derive a mean-field limit of a fermion system. Motivated by the method of the  $\alpha$  counting operator for bosonic systems, as introduced in [5], in this chapter, the method is adapted to a fermionic system.

The methods proceeds as follows: Suppose the system is described by some Slater determinant  $\Psi_N$ , which consists of one-particle wave functions  $\phi_j$ , of which some  $\phi'_j$  are not solutions of the Hartree-Fock equation. These  $\phi'_j$  are called bad particles. Because solutions of the Hartree-Fock equation imply a good mean-field approximation of the stationary system, the more bad particles are confined in  $\Psi_N$ , the worse a mean-field approximation is. But how does the number of bad particles develop, e.g. the quality of a mean-field approximation, as the system is observed in its time evolution and in the mean-field limit  $N \rightarrow \infty$ ?

Let  $\alpha^t$  be the relative number of bad particles at some time  $t$ . Assuming, the mean-field limit exists for an initial state  $\Psi_N^0$ ,

$$\lim_{N \rightarrow \infty} \alpha^0 = 0 \quad (4.1)$$

it is to show that, for some time  $t$ :

$$\lim_{N \rightarrow \infty} \alpha^t = 0. \quad (4.2)$$

For proving (4.2) under the assumption (4.1), the Grønwall Lemma is applied.

Grønwall Lemma:

Let  $I = [t_0, t_1]$ . Suppose  $a : I \rightarrow \mathbb{R}$  and  $b : I \rightarrow \mathbb{R}$  are continuous, and suppose  $u : I \rightarrow \mathbb{R}$  is a non-negative continuous function on  $I$  and satisfies:

$$u'(t) \leq a(t)u(t) + b(t) \quad \text{for } t \in I$$

then

$$u(t) \leq u(t_0)e^{\int_{t_0}^t a(\tau)d\tau} + \int_{t_0}^t b(s)e^{\int_s^t a(\tau)d\tau} ds.$$

For the counting operator  $\alpha^t$ , this means that, if the time derivative of  $\alpha^t$  can be expressed by  $\alpha^t$  times a constant plus some constant, which converges to zero in the mean-field limit,  $\alpha^t$  is bounded by  $\alpha^0$  times some constant plus another constant, which converges to zero in the mean-field limit:

$$\partial_t \alpha^t \leq C\alpha^t + G, \quad \lim_{N \rightarrow \infty} G = 0 \quad (4.3)$$

$$\implies \lim_{N \rightarrow \infty} \alpha^t = 0$$

And therefore, it is justified to approximate the many particle interaction by interactions with a mean-field. For a bosonic system, this proof is shown in [5].

In this chapter, the counting operator  $\alpha$  and its derivative is derived and reduced to a sum of three terms. Unfortunately, this is where this thesis comes to an end, as estimating these three terms, to obtain the derivative of  $\alpha$  in form of (4.3), would exceed the extent of this thesis. Therefore, this chapter only presents an outline of the whole proof.

The estimates for the three terms, and therefore the end of this proof, can be found in [4].

## 4.1 The counting operator $\alpha$

The aim of this chapter is to develop an operator which counts the relative number of bad particles in  $\Psi_N$ . Bad particles are one-particle wave functions of the Slater determinant  $\Psi_N$ , that are not the solution of the Hartree-Fock equations (3.6). Let  $\{\phi_j\}_{1 \leq j \leq N}$  be solutions of the Hartree-Fock equations, then

$$p_i^{\phi_j} = \langle \phi_j(x_i), \cdot \rangle \phi_j(x_i)$$

$$p^{\phi_j} = \sum_{i=1}^N p_i^{\phi_j} = \sum_{i=1}^N \langle \phi_j(x_i), \cdot \rangle \phi_j(x_i)$$

$p^{\phi_j}$  is a projector, that projects the j-th state of the Slater-determinant onto the j-th solution of the Hartree-Fock equations for all its coordinates. Let  $\phi'_j$  be a one-particle wave function of  $\Psi_N$ , and assuming  $\langle \phi_j, \phi'_j \rangle = 0$ , if  $\phi'_j$  is no solution of the Hartree-Fock equation.  $p^{\phi_j}$  applied to  $\Psi_N$  leads to:

$$p^{\phi_j} \Psi_N = \begin{cases} \Psi_N & , \text{if } \phi_j \text{ solution of HF} \\ 0 & , \text{otherwise} \end{cases}$$

For an example of how  $p^{\phi_j}$  is applied to a two-particle system, see example "Example of  $p^{\phi_j}$  applied to  $\Psi_2$ ", p. 31. The orthogonal projector of  $p^{\phi_j}$  is:

$$q^{\phi_j} = (1 - p^{\phi_j})$$

$$q^{\phi_j} \Psi_N = (1 - p^{\phi_j}) \Psi_N = \begin{cases} 0 & , \text{if } \phi_j \text{ solution of HF} \\ \Psi_N & , \text{otherwise} \end{cases}$$

With these projectors, the counting operator can be defined as:

$$\alpha(\Psi_N, \phi) = \frac{1}{N} \sum_{j=1}^N \langle \Psi_N, q^{\phi_j} \Psi_N \rangle \quad (4.4)$$

The terms of the sum are either 1 or 0, depending on whether  $\phi'_j$  is a bad particle or a good particle. Defining a new set of projectors, (4.4) can be simplified.

$$p_i = \sum_{j=1}^N p_i^{\phi_j} = \sum_{j=1}^N \langle \phi_j(x_i), \cdot \rangle \phi_j(x_i) \quad (4.5)$$

$$q_i = 1 - p_i \quad (4.6)$$

Applying (4.6) and (4.5) to the counting operator (4.4), leads to:

$$\begin{aligned} \alpha(\Psi_N, \phi) &= \frac{1}{N} \sum_{j=1}^N \langle \Psi_N, q^{\phi_j} \Psi_N \rangle = 1 - \frac{1}{N} \sum_{j=1}^N \langle \Psi_N, p^{\phi_j} \Psi_N \rangle \\ &= 1 - \frac{1}{N} \sum_{i,j=1}^N \langle \Psi_N, p_i^{\phi_j} \Psi_N \rangle = 1 - \frac{1}{N} \sum_{i=1}^N \langle \Psi_N, p_i \Psi_N \rangle \\ &= \frac{1}{N} \sum_{i=1}^N \langle \Psi_N, q_i \Psi_N \rangle = \langle \Psi_N, q_1 \Psi_N \rangle \end{aligned}$$

, where in the last step, it is used, that the projector  $p_i$  checks on every state  $\phi'$  of  $\Psi_N$  of being good or bad, for the  $i$ -th coordinate. The property of an one-particle state  $\phi'$  of being good or bad doesn't depend on its coordinate and with  $\langle \Psi_N, q_i \Psi_N \rangle = \langle \Psi_N, q_i^2 \Psi_N \rangle = \langle q_i \Psi_N, q_i \Psi_N \rangle = \|q_i \Psi_N\|^2$  same for any  $i$ , the terms of the sum are all equal and it is sufficient to check every state in its first coordinate. From a practical point of view,  $p_i$  and  $q_i$  can be seen as filters:  $p_i \Psi_N$  ( $q_i \Psi_N$ ) has no bad (good) particles at  $x_i$ . Auxiliary calculation "Basic Properties of  $p_i$   $q_i$ ", p.31 shows, that  $p_i$  and  $q_i$  are indeed hermitian projectors and auxiliary calculation "Example of  $p_1$  applied to  $\Psi_3$ ", p. 31, gives an illustrative example of the filter property of  $p_1$  in a three-state system.

## 4.2 The time derivative of $\alpha$

This chapter demonstrates the calculation of the time derivative of  $\alpha$  and its upper bound. As well as that, it gives an interpretation of how good particles turn bad.

$$i\partial_t \Psi_N = H\Psi_N, \quad i\partial_t \phi_i = h_i^{HF} \phi_i$$

$$\begin{aligned} \partial_t \alpha(\Psi_n, \phi) &= \partial_t \langle \Psi_N, q_1 \Psi_N \rangle \\ &= \langle \partial_t \Psi_N, q_1 \Psi_N \rangle + \langle \Psi_N, q_1 \partial_t \Psi_N \rangle + \langle \Psi_N, (\partial_t q_1) \Psi_N \rangle \end{aligned} \quad (4.7)$$

Calculating the first two terms separately from the last term and using the Schrödinger equation (2.13) and the Hartree-Fock equation (3.6) leads to:

$$\begin{aligned} \langle \partial_t \Psi_N, q_1 \Psi_N \rangle + \langle \Psi_N, q_1 \partial_t \Psi_N \rangle &= \langle -iH\Psi_N, q_1 \Psi_N \rangle + \langle \Psi_N, q_1 (-i)H\Psi_N \rangle \\ &= i \langle \Psi_N, Hq_1 \Psi_N \rangle - i \langle \Psi_N, q_1 H\Psi_N \rangle = i \langle \Psi_N, [H, q_1] \Psi_N \rangle \end{aligned} \quad (4.8)$$

$$\begin{aligned}
\partial_t q_1 &= \partial_t(1 - p_1) = -\partial_t \sum_{j=1}^N p_1^{\phi_j} \stackrel{BK}{=} -\sum_{j=1}^N \partial_t |\phi_j(x_1) \rangle \langle \phi_j(x_1)| \\
&= -\sum_{j=1}^N \{ \partial_t (|\phi_j(x_1) \rangle \langle \phi_j(x_1)| + |\phi_j(x_1) \rangle \partial_t \langle \phi_j(x_1)|) \} \\
&= -\sum_{j=1}^N \{ -i h_1^{HF} |\phi_j(x_1) \rangle \langle \phi_j(x_1)| + i |\phi_j(x_1) \rangle \langle \phi_j(x_1)| h_1^{HF} \} \quad (4.9) \\
&= -i \sum_{j=1}^N \{ -h_1^{HF} p_1^{\phi_j} + p_1^{\phi_j} h_1^{HF} \} = i \sum_{j=1}^N [h_1^{HF}, p_1^{\phi_j}] \\
&= i \left[ h_1^{HF}, \sum_{j=1}^N p_1^{\phi_j} \right] = i [h_1^{HF}, p_1] = -i [h_1^{HF}, q_1]
\end{aligned}$$

, where BK denotes a change to the Bra-Ket formalism. Using (4.8) and (4.9) in (4.7):

$$\begin{aligned}
\partial_t \alpha(\Psi_N, \phi) &= i \langle \Psi_N, [H, q_1] \Psi_N \rangle - i \langle \Psi_N, [h_1^{HF}, q_1] \Psi_N \rangle \\
&= i \langle \Psi_N, [H - h_1^{HF}, q_1] \Psi_N \rangle
\end{aligned}$$

$$\text{with } H = \sum_{i=1}^N h^{(i)} + \sum_{1 \leq i < j \leq N} v_N^\beta(x_i - x_j), \quad h_1^{HF} = h^{(1)} + v_{mf}^\beta(x_1)$$

$v_{mf}^\beta(x_1)$  describes the mean-field term of the Hartree-Fock equation. As stated before, it is justified to neglect the exchange term. Comparing  $H$  and  $h_1^{HF}$  in their the first coordinate, the non-interacting term,  $h^{(1)}$  cancels. Separating the terms, that don't depend on  $x_1$ , leads to:

$$\begin{aligned}
\partial_t \alpha(\Psi_N, \phi) &= i \left\langle \Psi_N, \left[ \sum_{k=2}^N v_N^\beta(x_k - x_1) - v_{mf}^\beta, q_1 \right] \Psi_N \right\rangle \\
&\quad + i \left\langle \Psi_N, \left[ \sum_{i=2}^N h^{(i)} + \sum_{2 \leq i < j \leq N} v_N^\beta(x_k - x_i), q_1 \right] \Psi_N \right\rangle
\end{aligned}$$

The second term vanishes as  $q_1$  commutes with  $\sum_{i=2}^N h^{(i)}$  and  $\sum_{2 \leq i < j \leq N} v_N^\beta(x_k - x_i)$

and due to the symmetry of  $\Psi_N$ , the terms of the first scalar product are all same:

$$\begin{aligned}
\partial_t \alpha(\Psi_N, \phi) &= i \left\langle \Psi_N, \left[ (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1), q_1 \right] \Psi_N \right\rangle \\
&= i \left\langle \Psi_N, \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 \Psi_N \right\rangle \\
&\quad - i \left\langle \Psi_N, q_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) \Psi_N \right\rangle \\
&= i \left\langle \Psi_N, (p_1 + q_1) \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 \Psi_N \right\rangle \\
&\quad - i \left\langle \Psi_N, q_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) (p_1 + q_1) \Psi_N \right\rangle \\
&= i \left\langle \Psi_N, q_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 \Psi_N \right\rangle \\
&\quad + i \left\langle \Psi_N, p_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 \Psi_N \right\rangle \\
&\quad - i \left\langle \Psi_N, q_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 \Psi_N \right\rangle \\
&\quad - i \left\langle \Psi_N, q_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) p_1 \Psi_N \right\rangle \\
&= i \left\langle \Psi_N, p_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 \Psi_N \right\rangle \\
&\quad - i \left\langle \Psi_N, q_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) p_1 \Psi_N \right\rangle \\
&= i \left\{ \left\langle \Psi_N, p_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 \Psi_N \right\rangle \right. \\
&\quad \left. - \left\langle p_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 \Psi_N, \Psi_N \right\rangle \right\} \\
&= i \left\{ \left\langle \Psi_N, p_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 \Psi_N \right\rangle \right. \\
&\quad \left. - \left\langle \Psi_N, p_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 \Psi_N \right\rangle^* \right\} \\
&= 2i \text{Im} \left\{ \left\langle \Psi_N, p_1 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 \Psi_N \right\rangle \right\} \\
&= 2i \text{Im} \left\{ \left\langle \Psi_N, p_1(p_2 + q_2) \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1(p_2 + q_2) \Psi_N \right\rangle \right\} \\
&= 2i \text{Im} \left\{ \left\langle \Psi_N, p_1 p_2 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 p_2 \Psi_N \right\rangle \right. \\
&\quad + \left\langle \Psi_N, p_1 p_2 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 q_2 \Psi_N \right\rangle \\
&\quad + \left\langle \Psi_N, p_1 q_2 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 p_2 \Psi_N \right\rangle \\
&\quad \left. + \left\langle \Psi_N, p_1 q_2 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 q_2 \Psi_N \right\rangle \right\}
\end{aligned} \tag{4.10}$$

The third term is equal to zero:

$$\begin{aligned}
& \left\langle \Psi_N, p_1 q_2 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 p_2 \Psi_N \right\rangle \\
&= (N-1) \left\langle \Psi_N, p_1 q_2 v_N^\beta(x_2 - x_1) q_1 p_2 \Psi_N \right\rangle - \left\langle \Psi_N, p_1 q_2 v_{mf}^\beta(x_1) q_1 p_2 \Psi_N \right\rangle \\
&= (N-1) \left\langle p_2 q_1 v_N^\beta(x_2 - x_1) q_2 p_1 \Psi_N, \Psi_N \right\rangle - \left\langle \Psi_N, p_1 v_{mf}^\beta(x_1) q_2 p_2 q_1 \Psi_N \right\rangle \\
&= (N-1) \left\langle \Psi_N, p_2 q_1 v_N^\beta(x_2 - x_1) q_2 p_1 \Psi_N \right\rangle^* \\
&= (N-1) \left\langle \Psi_N, p_1 q_2 v_N^\beta(x_2 - x_1) q_1 p_2 \Psi_N \right\rangle^*
\end{aligned}$$

Where it is used, that the mean-field potential  $v_{mf}(x_1)$  and  $q_1$  commute with  $q_2$ . That leads to a state being projected with  $p_2$  first and then with  $q_2$  afterwards, what is equal to zero. For the interaction term, it is used, that the interaction potential  $v_N^\beta(x_1 - x_2)$  is spherical symmetric, to show that this term is equal to its complex conjugated. That implies, that its imaginary part is zero.

Similarly, due to the commutation properties, the mean-field term in the second term of (4.10) vanishes. Therefore, (4.10) can be written as:

$$\begin{aligned}
\partial_t \alpha(\Psi_N, \phi) &= 2i \text{Im} \left\{ \left\langle \Psi_N, p_1 p_2 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 p_2 \Psi_N \right\rangle \right. \\
&\quad + \left\langle \Psi_N, p_1 p_2 (N-1)v_N^\beta(x_2 - x_1) q_1 q_2 \Psi_N \right\rangle \\
&\quad \left. + \left\langle \Psi_N, p_1 q_2 \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 q_2 \Psi_N \right\rangle \right\} \\
&\hspace{15em} (4.11)
\end{aligned}$$

At this point, a physical interpretation of the three terms above can be given. When observing the system for some time, due to the interaction term, particles will correlate and get entangled. Rewriting (4.11) gives:

$$\begin{aligned}
\partial_t \alpha(\Psi_N, \phi) &= 2i \text{Im} \left\{ \left\langle p_2 p_1 \Psi_N, \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 p_2 \Psi_N \right\rangle \right. \\
&\quad + \left\langle p_2 p_1 \Psi_N, (N-1)v_N^\beta(x_2 - x_1) q_1 q_2 \Psi_N \right\rangle \\
&\quad \left. + \left\langle q_2 p_1 \Psi_N, \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 q_2 \Psi_N \right\rangle \right\}
\end{aligned}$$

The first term can be seen as the overlap of a state with only good particles at  $x_1$  and  $x_2$ ,  $p_1 p_2 \Psi_N$ , with another state with only good particles at  $x_2$  and with a bad particle at  $x_1$ ,  $q_1 p_2 \Psi_N$ , which is subjected to the potentials  $v_N^\beta$  and  $v_{mf}^\beta$ . As defined in (4.5) and visualized in the example "Example of  $p_1$  applied to  $\Psi_3$ ", p. 31,  $p_i$  removes bad particles at  $x_i$ . But that doesn't imply bad particles can't exist at some other coordinates. Heuristically, the contribution to the derivative of  $\alpha$  could be explained by the transformation of good particles to bad particles at  $x_2$ , due to the interactions.

Similarly, the second term is the overlap of a state with good particles at  $x_1$  and  $x_2$  with a state with only bad particles at  $x_1$  and  $x_2$ , subjected to the two

particle interaction only. Because there is no good (bad) particle interacting with another good (bad) particle, there's no mean-field interaction appearing in this term. It could be described by particles becoming bad in both coordinates, due to the interaction.

The third term describes particles becoming bad as a result of the interactions potentials acting on a state with only good particles at  $x_1$  and with only bad particles at  $x_2$ . Interestingly, the mean-field term appears for the interaction of two bad particles.

As mentioned before, estimates of all three terms above are not presented in this thesis. But as the third term is comparably easy to estimate under some assumptions, it might still give an idea of how this proof may come to an end:

Assuming  $v_{mf}^\beta(x_1)$  and  $p_1(v_N^\beta(x_2 - x_1))^2 p_1$  are bounded by  $C_1$  and  $C_2^2$ , respectively:

$$\|v_{mf}^\beta(x_1)\|_{op} \leq C_1 \quad , \quad \|p_1((N-1)v_N^\beta(x_2 - x_1))^2 p_1\|_{op}^{\frac{1}{2}} \leq C_2$$

$$\begin{aligned} \left\langle q_2 p_1 \Psi_N, v_{mf}^\beta(x_1) q_1 q_2 \Psi_N \right\rangle &\leq \|q_2 p_1 \Psi_N\| \quad \|v_{mf}^\beta(x_1) q_1 q_2 \Psi_N\| \\ &= \|q_2 p_1 \Psi_N\| \quad \|q_1 q_2 \Psi_N\| \quad \|v_{mf}^\beta(x_1)\|_{op} \leq C_1 \|p_1\|_{op} \|q_1\|_{op} \|q_2 \Psi_N\|^2 \\ &= \alpha(\Psi_N, \phi) C_1 \end{aligned}$$

$$\begin{aligned} \left\langle q_2 p_1 \Psi_N, (N-1)v_N^\beta(x_2 - x_1) q_1 q_2 \Psi_N \right\rangle &\leq \|(N-1)v_N^\beta(x_2 - x_1) q_2 p_1 \Psi_N\| \quad \|q_1 q_2 \Psi_N\| \\ &= \leq \|p_1((N-1)v_N^\beta(x_2 - x_1))^2 p_1\|_{op}^{\frac{1}{2}} \quad \|q_2 \Psi_N\|^2 \leq \alpha(\Psi_N, \phi) C_2 \end{aligned}$$

With these two estimates, the third term can be estimated with:

$$\left\langle q_2 p_1 \Psi_N, \left( (N-1)v_N^\beta(x_2 - x_1) - v_{mf}^\beta(x_1) \right) q_1 q_2 \Psi_N \right\rangle \leq \alpha(\Psi_N, \phi) (C_2 - C_1)$$

This is the desired form of (4.3), to which the Grönwall Lemma is applicable and a mean-field approximation can be justified with.





## 5 Auxiliary calculations and examples

### Scalings

#### Fourier transformation of Coulomb potential

$$\begin{aligned}
 \int_{\mathbb{R}^3} dx' e^{i\langle k_i - k_j, x' \rangle} \frac{1}{\|x'\|} &= \lim_{\beta \rightarrow 0} \int_{\mathbb{R}^3} dx' e^{i\langle k_i - k_j, x' \rangle} e^{\beta \|x'\|} \frac{1}{\|x'\|} \\
 &= \lim_{\beta \rightarrow 0} \int_0^\infty \int_0^{2\pi} \int_0^\pi dr d\varphi d\vartheta \quad r^2 \sin \vartheta \frac{1}{r} e^{i\|k_i - k_j\| r \cos \vartheta} e^{\beta r} \\
 &\quad \text{substituting } t = \cos \vartheta, dt = -\frac{1}{\sin \vartheta} d\vartheta \\
 &= \lim_{\beta \rightarrow 0} 2\pi \int_0^\infty \int_{-1}^1 dr dt \quad r e^{i\|k_i - k_j\| r t} e^{\beta r} \\
 &= \lim_{\beta \rightarrow 0} 2\pi \int_0^\infty dr \quad r \frac{e^{i\|k_i - k_j\| r} - e^{-i\|k_i - k_j\| r}}{i\|k_i - k_j\| r} e^{\beta r} \\
 &= \lim_{\beta \rightarrow 0} \frac{4\pi}{\|k_i - k_j\|} \int_0^\infty dr \sin(\|k_i - k_j\| r) e^{\beta r} \\
 &\quad \text{the Fourier sinus transformation of } e^{\beta r} \text{ can be looked up} \\
 &= \lim_{\beta \rightarrow 0} \frac{4\pi}{\|k_i - k_j\|} \frac{\|k_i - k_j\|}{\|k_i - k_j\|^2 + \beta^2} = \frac{4\pi}{\|k_i - k_j\|^2}
 \end{aligned}$$

#### order in N of the convolution

using  $\|\phi_i\|^2 = \frac{1}{V}, V = V_0 N$  and estimating the Coulomb potential for  $x_2 = 0$ :

$$\int_{[0,L]^3} dx_1 \frac{1}{\|x_1 - x_2\|} \sum_{i=1}^N |\phi_i|^2 \leq \frac{1}{V_0} \int_{[0,L]^3} dx_1 \frac{1}{\|x_1\|}$$

The Coulomb potential is easier to integrate in spherical coordinates. As this is an estimate, it is justified to integrate over a sphere instead of a box.

$$\leq \frac{4\pi}{V_0} \int_0^{(V_0 N)^{\frac{1}{3}}} r^2 \frac{1}{r} dx_r = \frac{2\pi}{V_0^{\frac{1}{3}}} N^{\frac{2}{3}}$$

### Hartree-Fock equations

#### Lagrange multipliers $e_{ij}$ are diagonalizable

$$\delta L = \delta \langle \Psi, H \Psi \rangle - \sum_{i=1}^N \sum_{j=1}^N e_{ij} \delta \langle \phi_i, \phi_j \rangle \quad (5.1)$$

as  $\delta L$  is real, the  $e_{ij}$  are hermitian:

$$\begin{aligned}\delta L - \delta L^* &= - \sum_{i=1}^N \sum_{j=1}^N e_{ij} \delta \langle \phi_i, \phi_j \rangle + \sum_{i=1}^N \sum_{j=1}^N e_{ij}^* (\delta \langle \phi_i, \phi_j \rangle)^* \\ &= \sum_{i=1}^N \sum_{j=1}^N [e_{ji}^* - e_{ij}] \delta \langle \phi_i, \phi_j \rangle = 0\end{aligned}$$

From this follows, that  $e_{ji}^* = e_{ij}$ , e.g.  $e_{ij}$  is hermitian. Let  $S$  define a change of a basis:

$$\phi'_j = \sum_{i=1}^N \phi_i S_{ij} \quad , \quad \Psi'_N = (\det S) \Psi'_N$$

As  $S$  is unitary, its determinant is equal to one. Therefore, the mean energy does not change due to the change of basis:

$$\delta L = \delta \langle \Psi, H \Psi \rangle - \sum_{k=1}^N \sum_{l=1}^N e'_{kl} \delta \langle \phi'_k, \phi'_l \rangle$$

Applying the one particle wave functions to variation function above and defining  $e_{ij} = (S^\dagger e' S)_{ij}$  leads to equation (5.1).  $S$  can be chosen in a way, that diagonalizes  $e'$ .

### Simplifying the complex conjugated term of the variation equation

$$\begin{aligned}c.c. &= \sum_{i=1}^N \langle \phi_i, h^{(i)} \delta \phi_i \rangle + \sum_{i=1}^N \sum_{j=1}^N \left\{ \langle \phi_i \phi_j, v_{12}^\beta \delta \phi_i \phi_j \rangle - \langle \phi_i \phi_j, v_{12}^\beta P_{ij} \delta \phi_i \phi_j \rangle \right\} \\ &\quad - \sum_{i=1}^N e_i \langle \phi_i, \delta \phi_i \rangle \\ &= \sum_{i=1}^N \int dx_1 \left[ h^{(i)} \phi_i^*(x_1) + \sum_{j=1}^N \int dx_2 \phi_i^*(x_1) \phi_j^*(x_2) v_{12}^\beta \phi_j(x_2) \right. \\ &\quad \left. - \sum_{j=1}^N \int dx_2 \phi_j^*(x_2) \phi_i^*(x_1) v_{12}^\beta P_{ij} \phi_j(x_2) - e_i \phi_i^*(x_1) \right] \delta \phi_i(x_1) \\ &= \sum_{i=1}^N \int dx_1 \phi_i^*(x_1) \left[ h^{(i)} + \sum_{j=1}^N \int dx_2 \phi_j^*(x_2) v_{12}^\beta \phi_j(x_2) \right. \\ &\quad \left. - \sum_{j=1}^N \int dx_2 \phi_j^*(x_2) v_{12}^\beta P_{ij} \phi_j(x_2) - e_i \right] \delta \phi_i(x_1)\end{aligned}$$

## The counting operational $\alpha$

### Example of $p^{\phi_j}$ applied to $\Psi_2$

(neglecting the normalization factor  $\frac{1}{\sqrt{2}}$ ):

$$\Psi(x_1, x_2) = \phi'_1(x_1)\phi'_2(x_2) - \phi'_1(x_2)\phi'_2(x_1)$$

$\phi_2$  is checked of being good or bad:

$$\begin{aligned} p^{\phi_2}\Psi(x_1, x_2) &= \sum_{i=1}^2 \langle \phi_2(x_i), \Psi(x_1, x_2) \rangle \phi_2(x_i) \\ &= \langle \phi_2(x_1), \phi'_1(x_1)\phi'_2(x_2) - \phi'_1(x_2)\phi'_2(x_1) \rangle \phi_2(x_1) \\ &\quad + \langle \phi_2(x_2), \phi'_1(x_1)\phi'_2(x_2) - \phi'_1(x_2)\phi'_2(x_1) \rangle \phi_2(x_2) \\ &= \langle \phi_2(x_1), \phi'_1(x_2) \rangle \phi_2(x_2)\phi_2(x_1) - \langle \phi_2(x_1), \phi'_1(x_1) \rangle \phi_1(x_2)\phi_2(x_1) \\ &\quad + \langle \phi_2(x_2), \phi'_1(x_2) \rangle \phi_1(x_1)\phi_2(x_2) - \langle \phi_2(x_2), \phi'_1(x_1) \rangle \phi_2(x_1)\phi_2(x_2) \\ &= \delta_{\phi_2\phi'_2} \{ \phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1) \} = \delta_{\phi_2\phi'_2} \Psi(x_1, x_2) \end{aligned}$$

### Basic Properties of $p_i$ $q_i$

Since  $p_i^{\phi_j}$  and  $q_i^{\phi_j}$  are projectors (hermitian),

$$p_i^2 = \left( \sum_{j=1}^N p_i^{\phi_j} \right)^2 = \sum_{j=1}^N \left( p_i^{\phi_j} \right)^2 + 2 \sum_{1 \leq l < k \leq N} p_i^{\phi_l} p_i^{\phi_k} = \sum_{j=1}^N p_i^{\phi_j} = p_i$$

$p_i$  is a projector as well. Similarly, one can show that  $q_i$  is a projector.

$p_i$  and  $q_i$  are hermitian:

$$p_i^\dagger = \left( \sum_{j=1}^N p_i^{\phi_j} \right)^\dagger = \sum_{j=1}^N \left( p_i^{\phi_j} \right)^\dagger = \sum_{j=1}^N p_i^{\phi_j} = p_i$$

### Example of $p_1$ applied to $\Psi_3$

(neglecting the normalization factor  $\frac{1}{6}$ ):

$$\begin{aligned} \Psi_3 &= \phi_1(x_1)\phi_2(x_2)\phi_3(x_3) + \phi_1(x_2)\phi_2(x_3)\phi_3(x_1) + \phi_1(x_3)\phi_2(x_1)\phi_3(x_2) \\ &\quad - \phi_1(x_3)\phi_2(x_2)\phi_3(x_1) - \phi_1(x_2)\phi_2(x_1)\phi_3(x_3) - \phi_1(x_1)\phi_2(x_3)\phi_3(x_2) \end{aligned}$$

assuming,  $\phi_3$  is bad:

$$\begin{aligned} p_1\Psi_3 &= \phi_1(x_1)\phi_2(x_2)\phi_3(x_3) + \phi_1(x_3)\phi_2(x_1)\phi_3(x_3) \\ &\quad - \phi_1(x_2)\phi_2(x_1)\phi_3(x_3) - \phi_1(x_1)\phi_2(x_2)\phi_3(x_3) \\ &= \{ \phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1) \} \phi_3(x_3) \\ &\quad + \{ \phi_1(x_3)\phi_2(x_1) - \phi_1(x_1)\phi_2(x_3) \} \phi_3(x_2) \end{aligned}$$

The projector acts on every state at  $x_1$ . As only  $\phi_3$  is bad, only projections acting on  $\phi_3(x_1)$  cancel out. This example illustrates, how  $p_1$  only filters bad particles at  $x_1$  but generally leaves bad particles at other coordinates behind.



## 6 Bibliography

- [1] B Schlein H. T. Yau A. Elgart L. Erdős. “Nonlinear Hartree equation as the mean field limit of weakly coupled fermions”. In: (2003).
- [2] H.Bethe A. Sommerfeld. *Elektronentheorie der Metalle*. Springer, 1967.
- [3] B. Schlein N. Benedikter M. Porta. “Mean-field Evolution of Fermionic Systems”. In: *arXiv:1305.2768* (2013).
- [4] Petrat/Pickl. “Derivation of mean-field dynamics for fermions. In preparation”. In: (2014).
- [5] Peter Pickl. “A simple derivation of mean field limits for quantum systems”. In: *arXiv:0907.4464* (2011).



# Erklärung

Ich erkläre hiermit, dass ich die vorliegende Arbeit selbstständig und nur mithilfe der angegebenen Quellen angefertigt habe. Alle Zitate habe ich solche kenntlich gemacht.

Datum, Unterschrift