
Mean-field quantum dynamics with magnetic fields

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Chapter 1

Introduction

The aim of this thesis is to investigate the mean-field quantum dynamics of boson systems subject to an external magnetic field. We will outline three different approaches to mean-field quantum dynamics and present our results on how to adapt these methods to include a magnetic field.

1.1 Quantum mechanics of many-body systems

A quantum mechanical system of N particles in d dimensions can be described by a complex-valued wave function $\psi_N(x_1, \dots, x_N) \in L^2(\mathbb{R}^{Nd})$ with the normalisation condition $\|\psi_N\|_2 = 1$. The position of the j -th particle is denoted by $x_j \in \mathbb{R}^d$ for $j \in \{1, \dots, N\}$. The square of the modulus of the wave function, $|\psi_N(x_1, \dots, x_N)|^2$, can be interpreted as the probability of finding the first particle at position x_1, \dots , and the N -th particle at position x_N .

There are two different types of particles in Nature: bosons and fermions. The wave function of N indistinguishable bosons is symmetric with respect to permutations of the variables, i.e.

$$\psi_N(x_{\pi(1)}, x_{\pi(2)}, \dots, x_{\pi(N)}) = \psi_N(x_1, x_2, \dots, x_N) \quad (1.1)$$

for all permutations π of $\{1, 2, \dots, N\}$. In contrast, the wave function of N indistinguishable fermions is antisymmetric with respect to permutations of the variables, i.e.

$$\psi_N(x_{\pi(1)}, x_{\pi(2)}, \dots, x_{\pi(N)}) = (-1)^{\text{sgn } \pi} \psi_N(x_1, x_2, \dots, x_N) \quad (1.2)$$

for all permutations π of $\{1, 2, \dots, N\}$, where $\text{sgn } \pi$ denotes the sign of the permutation π .

Physical observables are given by self-adjoint operators A on $L^2(\mathbb{R}^{Nd})$. If the system is in the state ψ_N , the expectation value of a measurement with the observable A is given by

$$\langle \psi_N, A\psi_N \rangle = \int_{\mathbb{R}^{Nd}} dx_1 \dots dx_N \overline{\psi_N}(x_1, \dots, x_N) (A\psi_N)(x_1, \dots, x_N). \quad (1.3)$$

For example, the multiplication operator x_j is the observable measuring the position of the j -th particle and the differential operator $-i\nabla_{x_j}$ is the observable measuring the momentum of the j -th particle.

The time evolution of the system is governed by the Schrödinger equation

$$\begin{cases} i\partial_t\psi_{N,t} = H_N\psi_{N,t}, \\ \psi_{N,t=0} = \psi_N, \end{cases} \quad (1.4)$$

in which $\psi_{N,t}$ denotes the wave function of the system at time t , H_N is the Hamiltonian of the system and ψ_N is the initial state of the system at time $t = 0$. Here and henceforth, the subscript t to a quantity denotes its time-dependence.

The Hamiltonian H_N is the energy observable of the system. For a many-body system with two-particle interactions, it has the form

$$H_N = \sum_{j=1}^N (h_j + U_{\text{ext}}(x_j)) + \lambda \sum_{i<j}^N V(x_i - x_j). \quad (1.5)$$

The first part of the Hamiltonian is a sum of one-particle operators where the sum over the one-particle operators h_j is the kinetic part of the Hamiltonian. The function $U_{\text{ext}} : \mathbb{R}^d \rightarrow \mathbb{R}$ is an external potential acting on every particle in the same way. It describes for example a confining potential which traps the particles in a certain region. The second part of the Hamiltonian is a sum over all pairs of particles and the interaction between the particles is described by the potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$. $\lambda \in \mathbb{R}$ is a coupling constant.

For non-relativistic quantum systems the kinetic energy operator is $h = -\Delta$. An external magnetic field is accounted for by taking $h = (-i\nabla + A(x))^2$ where $A : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is the magnetic vector potential. For systems where relativistic effects cannot be neglected, one typically adopts the semi-relativistic treatment by choosing $h = \sqrt{1 - \Delta}$.

Under appropriate conditions of h and V , the Hamiltonian H_N can be self-adjointly realised in $L^2(\mathbb{R}^{Nd})$. Then $\psi_{N,t} = e^{-iH_N t}\psi_N$ is the solution to the Schrödinger equation (1.4) by Stone's Theorem and there is conservation of mass and energy, i.e.

$$\|\psi_N\|_2 = \|\psi_{N,t}\|_2 \quad \text{and} \quad \langle \psi_N, H_N \psi_N \rangle = \langle \psi_{N,t}, H_N \psi_{N,t} \rangle \quad \text{for all } t \in \mathbb{R}. \quad (1.6)$$

1.2 Dynamical analysis in the mean-field regime

We are interested in the dynamics of a large system of N identical and spinless bosons in d dimensions. A typical real-world example for such a system is a dilute Bose-Einstein condensate which contains $N \sim 10^2 - 10^{10}$ atoms (see e.g. [25]).

In principle, the dynamics of the system is determined by solving the Schrödinger equation. Owing to the large particle numbers, it is practically impossible to derive an explicit solution. Also, numerical simulations are hopeless. However, one does not necessarily need to know the evolution of every particle in the system. Typical observables in experiments involve only a small number of particles, usually one or two. Therefore, the interest is rather towards macroscopic properties of the system which result from averaging over a large number of particles.

Throughout this thesis, we consider the description of (1.5) in the mean-field regime. This is a natural approximation which one usually adopts to obtain a first qualitative understanding of a many-body quantum system. It allows us to derive effective evolution equations which are on the one hand at least numerically solvable and which on the other hand give a very good approximate description of the macroscopic behaviour of the system. The mean-field Hamiltonian is given by

$$H_N = \sum_{j=1}^N h_j + \frac{1}{N} \sum_{i<j}^N V(x_i - x_j), \quad (1.7)$$

where h is the one-particle operator. The scaling $\frac{1}{N}$ in front of the potential describes very weak interactions among the particles. It also ensures that the kinetic and potential energy are of the same order in N . Moreover, we consider only a condensate as initial data, i.e.

$$\psi_N(x_1, \dots, x_N) = \prod_{j=1}^N \varphi(x_j) \quad (1.8)$$

for some $\varphi \in L^2(\mathbb{R}^d)$. These factorised states are of physical interest because they can approximately describe states close to the ground state of H_N . Physically, such a mean-field model could describe a dilute, cold Bose gas or a gravitating Boson star far away from collapse.

Since the initial data $\psi_N = \varphi^{\otimes N}$ is factorised and the interaction between the particles is only very weak, it is reasonable to expect that the wave function of the system will stay approximately factorised over the time evolution. That is, we expect in a sense to be made more precise later on, that also at time $t > 0$,

$$\psi_{N,t}(x_1, \dots, x_N) \simeq \prod_{j=1}^N \varphi_t(x_j) \quad (1.9)$$

for a one-particle wave function $\varphi_t \in L^2(\mathbb{R}^d)$. Note that this cannot hold as an identity for wave functions in $L^2(\mathbb{R}^{Nd})$ because the interaction creates correlations between the particles. Heuristically, when $\psi_{N,t}$ is essentially factorised as in (1.9), the particles are distributed independently in space with probability density $|\varphi_t|^2$. By the law of large numbers, one therefore expects that the total interaction potential experienced by a single particle at position x_i in the limit $N \rightarrow \infty$ will be

$$\frac{1}{N} \sum_{j \neq i}^N V(x_i - x_j) \simeq \frac{1}{N} \sum_{j \neq i}^N \int_{\mathbb{R}^d} V(x_i - y) |\varphi_t(y)|^2 dy \simeq (V * |\varphi_t|^2)(x_i). \quad (1.10)$$

This suggests that the one-particle wave function φ_t obeys the Hartree equation

$$\begin{cases} i\partial_t \varphi_t = h\varphi_t + (V * |\varphi_t|^2)\varphi_t, \\ \varphi_{t=0} = \varphi. \end{cases} \quad (1.11)$$

The main goal in the study of mean-field quantum dynamics is to prove rigorously that the limiting dynamics as $N \rightarrow \infty$ is indeed given by the solution φ_t to the Hartree equation. Unfortunately, we cannot expect that $\|\psi_{N,t} - \varphi_t^{\otimes N}\|_{L^2(\mathbb{R}^{Nd})} \rightarrow 0$ holds as $N \rightarrow \infty$. Simple examples show that this notion of convergence is too strong.

However, we already mentioned the good news that many physical observables only act on a smaller number of particles, say k particles, out of the overall N particles. In order to be able to predict the time evolution of the expectation value of measurements of such observables one actually does not need the “full information” contained in $\psi_{N,t}$. The appropriate objects which we have to introduce are density matrices and their k -particle marginals. These are suitable objects to describe macroscopic properties of the system. They will give rise to a weaker notion of “closeness” (1.9) and we will be able to prove that the limiting dynamics is determined by the solution φ_t to the Hartree equation in this weaker sense. The macroscopic properties of the system, computed in the limiting regime $N \rightarrow \infty$, are then expected to be a good approximation for the macroscopic properties observed in experiments, where the number of particles N is very large, but finite.

Let $\psi_N \in L^2(\mathbb{R}^{Nd})$, $\|\psi_N\|_2 = 1$, be the symmetric wave function of a state of N identical bosons. With ψ_N we associate the density matrix

$$\gamma_N := |\psi_N\rangle\langle\psi_N|, \quad (1.12)$$

i.e. the orthogonal projection onto the state ψ_N . The operator γ_N is a positive trace class operator on $L^2(\mathbb{R}^{Nd})$ with unit trace. These properties are more generally the definition of a density matrix.

As a trace class operator, γ_N has an integral kernel $\gamma_N(\mathbf{x}_N; \mathbf{x}'_N)$ which is given by

$$\gamma_N(\mathbf{x}_N; \mathbf{x}'_N) = \psi_N(\mathbf{x}_N) \overline{\psi_N(\mathbf{x}'_N)}. \quad (1.13)$$

For every $k \in \{1, \dots, N\}$ we also define the corresponding k -particle marginal density or reduced density matrix $\gamma_N^{(k)}$ as the partial trace over the last $(N - k)$ particles:

$$\gamma_N^{(k)} = \text{tr}_{[k+1, \dots, N]} \gamma_N. \quad (1.14)$$

One obtains the integral kernel of $\gamma_N^{(k)}$ by integrating out the last $(N - k)$ particles from the integral kernel of γ_N :

$$\gamma_N^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) = \int_{\mathbb{R}^{(N-k)d}} d\mathbf{x}_{N-k} \gamma_N(\mathbf{x}_k, \mathbf{x}_{N-k}; \mathbf{x}'_k, \mathbf{x}_{N-k}). \quad (1.15)$$

This last equation can be considered as the definition of the partial trace of a density matrix. It is easy to verify that $\gamma_N^{(k)}$ is then a density matrix on $L^2(\mathbb{R}^{kd})$. See [30] and [32] for a comprehensive account of the properties of trace class operators and integral kernels of operators. The precise definition of the partial trace is given in Appendix 8.1.

Here we use the notation: $\mathbf{x}_N = (x_1, \dots, x_N)$, $\mathbf{x}'_N = (x'_1, \dots, x'_N) \in \mathbb{R}^{Nd}$ and $\mathbf{x}_k = (x_1, \dots, x_k)$, $\mathbf{x}'_k = (x'_1, \dots, x'_k) \in \mathbb{R}^{kd}$ as well as $\mathbf{x}_{N-k} = (x_{k+1}, \dots, x_N) \in \mathbb{R}^{(N-k)d}$ with $x_j, x'_j \in \mathbb{R}^d$ for $j \in \{1, \dots, N\}$.

A system in the state ψ_N can equivalently be described in terms of the associated density matrix γ_N . The expectation value of a measurement with an observable A on the system is then given by

$$\langle\psi_N, A\psi_N\rangle = \text{tr} A\gamma_N. \quad (1.16)$$

Moreover, if $J^{(k)}$ is a k -particle operator we have for the expectation value of a measurement with $J^{(k)}$ on the N -particle system

$$\langle \psi_N, (J^{(k)} \otimes \mathbb{1}_{N-k}) \psi_N \rangle = \text{tr} (J^{(k)} \otimes \mathbb{1}_{N-k}) \gamma_N = \text{tr} J^{(k)} \gamma_N^{(k)}. \quad (1.17)$$

Note that on the right-hand side of (1.17) the trace is only taken over k particles. So in order to predict the outcome of a measurement with $J^{(k)}$ on the evolved system at a later time $t > 0$, it is enough to know the k -particle marginal density $\gamma_{N,t}^{(k)}$ associated with the wave function $\psi_{N,t}$ of the system at that time.

We argued above that we expect the limiting dynamics to be given by the solution φ_t to the Hartree equation (1.11). Therefore, we would hope to approximate $\gamma_{N,t}^{(k)}$ with $|\varphi_t\rangle\langle\varphi_t|^{\otimes k}$ in the limit $N \rightarrow \infty$. Since these operators are all of trace class, a natural norm for this approximation is the trace norm on the space $\mathcal{L}^1(L^2(\mathbb{R}^{kd}))$ of trace class operators on $L^2(\mathbb{R}^{kd})$. We would therefore hope to show that for every fixed $k \in \mathbb{N}$ and every fixed $t \in \mathbb{R}$,

$$\lim_{N \rightarrow \infty} \text{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right| = 0. \quad (1.18)$$

The study of mean-field quantum dynamics has a relatively long history. The first proof of the convergence (1.18) for non-relativistic systems with bounded interaction potentials was established by Spohn [37] in 1980. An overview of results on mean-field quantum dynamics is given in Section 1.4.

The following graphic illustrates the guiding principle of the effective description of mean-field quantum dynamics: By considering only the k -particle marginals associated with the state of a system one can approximate in the limit $N \rightarrow \infty$ the many-body linear dynamics with the one-body nonlinear Hartree dynamics. Note though that by passing from the density matrix γ_N to a reduced density matrix $\gamma_N^{(k)}$, one loses irreversibly information about the system.

$$\begin{array}{ccccccc} \psi_N & \longrightarrow & \gamma_N & \xrightarrow{\text{partial trace}} & \gamma_N^{(k)} & \equiv & |\varphi\rangle\langle\varphi|^{\otimes k} \\ \text{many-body} & & \downarrow & & \downarrow & & \downarrow \\ \text{linear dynamics} & & & & & & \text{one-body nonlinear} \\ & & & & & & \text{Hartree dynamics} \\ \psi_{N,t} & \longrightarrow & \gamma_{N,t} & \xrightarrow{\text{partial trace}} & \gamma_{N,t}^{(k)} & \xrightarrow{N \rightarrow \infty} & |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \end{array} \quad (1.19)$$

1.3 Our model: assumptions and main result

In this thesis we investigate the mean-field quantum dynamics with magnetic fields of a system of N identical and spinless bosons. We restrict the analysis to the physically relevant case of three dimensions. In the concluding remarks in Chapter 7 we also comment on other dimensions.

Throughout we will make the following assumption regarding the magnetic vector potential $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ and the generated magnetic field $B = \nabla \times A$:

Assumption (A). Let $A \in C^\infty(\mathbb{R}^3; \mathbb{R}^3)$ and define $B = \nabla \times A$. Assume that there exists

$\varepsilon > 0$ such that

$$\begin{aligned} |\partial^\alpha B(x)| &\leq C_\alpha (1 + |x|)^{-(1+\varepsilon)} & \forall |\alpha| \geq 1, \forall x \in \mathbb{R}^3, \\ |\partial^\alpha A(x)| &\leq C_\alpha & \forall |\alpha| \geq 1, \forall x \in \mathbb{R}^3, \end{aligned}$$

where C_α are constants depending only on the multi-index α .

For $A \in L^2_{loc}(\mathbb{R}^3; \mathbb{R}^3)$ we define the *magnetic Sobolev space* as

$$H^1_A(\mathbb{R}^3) = \{ \varphi \in L^2(\mathbb{R}^3) \mid (-i\nabla + A)\varphi \in L^2(\mathbb{R}^3) \}. \quad (1.20)$$

This allows us to state our strongest result.

Theorem 6.6. *Let $V \in L^\infty(\mathbb{R}^3)$ or $V(x) = \frac{\lambda}{|x|}$, $\lambda \in \mathbb{R}$, and assume that the magnetic vector potential $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ satisfies assumption **(A)**. We consider the mean-field quantum dynamics generated by the Hamiltonian*

$$H_N = \sum_{j=1}^N (-i\nabla_{x_j} + A(x_j))^2 + \frac{1}{N} \sum_{i < j}^N V(x_i - x_j). \quad (1.21)$$

Let $\varphi \in H^1_A(\mathbb{R}^3)$ with $\|\varphi\|_2 = 1$ and set $\psi_N = \varphi^{\otimes N}$. Let $\psi_{N,t} = e^{-iH_N t} \psi_N$ and denote by φ_t the solution to the initial value problem for the magnetic Hartree equation

$$\begin{cases} i\partial_t \varphi_t = (-i\nabla + A)^2 \varphi_t + (V * |\varphi_t|^2) \varphi_t, \\ \varphi_{t=0} = \varphi. \end{cases} \quad (1.22)$$

Denote by $\gamma_{N,t}^{(k)}$ the k -particle marginals associated with $\psi_{N,t}$. Then there exists a constant $C > 0$ such that, for $k \in \mathbb{N}$ and $t \in \mathbb{R}$,

$$\mathrm{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle \langle \varphi_t|^{\otimes k} \right| \leq 2 \sqrt{\frac{k}{N}} e^{Ct} \quad (1.23)$$

holds for all $N \geq k$. In particular, this implies for every fixed $k \in \mathbb{N}$ and every fixed $t \in \mathbb{R}$

$$\lim_{N \rightarrow \infty} \mathrm{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle \langle \varphi_t|^{\otimes k} \right| = 0. \quad (1.24)$$

1.4 A short history of known results

Unless stated otherwise, the following results refer to the case $h = -\Delta$.

The first results establishing a relation between the many-body Schrödinger evolution and the nonlinear Hartree dynamics for smooth interaction potentials V were obtained by Hepp in [23]. Ginibre and Velo generalised his results to singular potentials in [20] and [21]. Their work was inspired by techniques from quantum field theory.

The first proof of the convergence (1.18) for bounded potentials $V \in L^\infty(\mathbb{R}^d)$ was given by Spohn [37] in 1980. His method is based on expanding the BBGKY hierarchy of evolution equations for marginals. Since then, there has been a flourishing activity in research on

mean-field quantum dynamics. Progress has been made mainly in two directions: First, to show the convergence (1.18) for more singular potentials and second, to obtain estimates on the rate of convergence of (1.18).

In [12], Erdős and Yau generalised and extended Spohn's method to the Coulomb potential $V(x) = \frac{\lambda}{|x|}$, $\lambda \in \mathbb{R}$, which is of particular physical interest. Partial results in this direction had been obtained before by Bardos, Golse and Mauser (see [2] and [3]). The method was extended by Elgart and Schlein in [10] to the case of semi-relativistic energy, i.e. $h = \sqrt{1 - \Delta}$, and Coulomb interactions. This case is technically more demanding, because the kinetic and potential energy have the same scaling behaviour and the corresponding Hamiltonian is energy-critical.

A different approach to the non-relativistic case with Coulomb interactions was taken by Fröhlich, Knowles and Schwarz in [18]. Their proof of (1.18) relies on dispersive estimates and the counting of Feynman graphs.

Moreover, in [17] Fröhlich, Graffi and Schwarz consider for smooth potentials the mean-field limit uniformly in Planck's constant \hbar . This allows them to combine the semi-classical limit and the mean-field limit.

In [33], Rodnianski and Schlein proved the convergence (1.18) for Coulomb interactions using an idea of Hepp [23]. They obtained an estimate on the rate of convergence of the type:

$$\mathrm{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right| \leq \frac{C(k)}{\sqrt{N}} e^{K(k)t}, \quad (1.25)$$

where $C(k), K(k) > 0$ are k -dependent constants.

Under the more restrictive conditions that the interaction potential V is bounded and has an integrable Fourier transform, Erdős and Schlein proved in [11] a better estimate on the rate of convergence:

$$\mathrm{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right| \leq C_1 \frac{k^2}{N} e^{C_2 k} e^{C_3 t} \quad (1.26)$$

for some constants $C_1, C_2, C_3 > 0$.

More recently, Knowles and Pickl took yet another approach to show the convergence (1.18). By considering a different, but equivalent indicator for the convergence (1.18) they were able to derive estimates on the rate of convergence for more singular potentials. For instance in the non-relativistic case in three dimensions, they obtain for singularities at the origin up to, but not including, the type $1/|x|^{3/2}$, the estimate:

$$\mathrm{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right| \leq 2\sqrt{\frac{k}{N}} e^{Ct} \quad (1.27)$$

for some constant $C > 0$. Their method can also treat the semi-relativistic case and it can be extended to even more singular potentials.

Parallel to the above investigations on the mean-field regime for many-body quantum systems, a further analysis was carried out to deal with more realistic hard-core, short-range interactions. This translates into a modification of the interaction term in the Hamiltonian (1.7). One replaces the mean-field potential $\frac{1}{N}V(x)$ with a term of the form $\frac{1}{N}V_N(x)$, where

V_N converges to a delta-interaction potential as $N \rightarrow \infty$. The emerging one-body effective description is then given by the nonlinear Gross-Pitaevskii equation

$$\begin{cases} i\partial_t\varphi_t = -\Delta\varphi_t + \sigma|\varphi_t|^2\varphi_t, \\ \varphi_{t=0} = \varphi, \end{cases} \quad (1.28)$$

for some $\sigma \in \mathbb{R}$. Notice that the Gross-Pitaevskii equation (1.28) is formally obtained from the Hartree equation (1.11) with $h = -\Delta$ by inserting “ $V(x) = \sigma\delta(x)$ ”.

Although the general treatment of this model goes through the conceptual scheme presented in this thesis, genuinely new tools are needed to control the singular scaling of the delta-interaction. For a comprehensive overview of this subject we refer to the review [34].

1.5 Outline of the thesis

This thesis is organised as follows.

Chapter 2:

We study the relationship between two indicators for the factorisation of the k -particle marginals $\gamma_{N,t}^{(k)}$ in the limit $N \rightarrow \infty$. We also present an improved estimate (2.16).

Chapter 3:

We prove the global well-posedness of the magnetic Hartree equation for a fairly general class of magnetic vector potentials which includes the physically relevant case of a constant magnetic field. Its global well-posedness is an important prerequisite for the study of the mean-field quantum dynamics with magnetic fields in the subsequent chapters.

Chapter 4:

We use a method based on the perturbative expansion of the BBGKY hierarchy to study the mean-field quantum dynamics with magnetic fields for bounded interaction potentials in three dimensions. The method was introduced by Spohn in [37] and we present minor modifications in order to adapt it to the magnetic case.

Chapter 5:

Using a compactness argument based on the BBGKY hierarchy we study the mean-field quantum dynamics with magnetic fields for bounded interaction potentials in three dimensions. The method was developed by Bardos, Erdős, Golse, Mauser and Yau in [2], [3] and [12]. We present several non-trivial modifications, in particular Propositions 5.3, 5.6, 5.10 and 5.12, to adapt it to the magnetic case.

Chapter 6:

In the first part, we outline the projections method introduced by Knowles and Pickl in [24] for mean-field quantum dynamics in arbitrary dimension d . In the second part we apply their method to the case of mean-field quantum dynamics with magnetic fields in three dimensions for bounded potentials and also for the Coulomb potential.

1.6 Conventions and notation

A subscript t to a variable denotes the time-dependence of this variable.

We use the following abbreviations for the position variables: $\mathbf{x}_N = (x_1, \dots, x_N)$, $\mathbf{x}'_N = (x'_1, \dots, x'_N)$, $\mathbf{x}_k = (x_1, \dots, x_k)$, $\mathbf{x}'_k = (x'_1, \dots, x'_k)$ and $\mathbf{x}_{N-k} = (x_{k+1}, \dots, x_N)$ with $x_j, x'_j \in \mathbb{R}^d$ for $j \in \{1, \dots, N\}$. The dimension d is usually clear from the context. Also we use $\nabla_j \equiv \nabla_{x_j}$ and $\nabla'_j \equiv \nabla_{x'_j}$.

Let $h : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ be a one-particle operator, $N \in \mathbb{N}$ and $j \in \{1, \dots, N\}$. Then the operator h_j is always understood to act on an N -particle wave function in $L^2(\mathbb{R}^{Nd})$ as the operator $\mathbb{1}_1 \otimes \dots \otimes \mathbb{1}_{j-1} \otimes h_j \otimes \mathbb{1}_{j+1} \otimes \dots \otimes \mathbb{1}_N$.

Let $1 \leq p \leq \infty$. The conjugate exponent p' to p is defined through the relation $\frac{1}{p} + \frac{1}{p'} = 1$.

The symbols C, C' stand for generic positive constants that may depend on some fixed parameters; their concrete value may change in the course of an estimate.

List of symbols:

\mathcal{H}	a Hilbert space
$\langle \cdot, \cdot \rangle$	the scalar product of a Hilbert space, linear in the second argument
X, Y	Banach spaces
$X \hookrightarrow Y$	$X \subset Y$ with continuous injection
$L^p(\mathbb{R}^d) \equiv L^p$	the space of functions $f : \mathbb{R}^d \rightarrow \mathbb{C}$ such that $\ f\ _{L^p(\mathbb{R}^d)} < \infty$, where $\ f\ _{L^p(\mathbb{R}^d)} = \begin{cases} \left(\int_{\mathbb{R}^d} dx f(x) ^p \right)^{\frac{1}{p}} & \text{if } 1 \leq p < \infty, \\ \text{ess sup}_{x \in \mathbb{R}^d} f(x) & \text{if } p = \infty. \end{cases}$
$\ \cdot\ _p$	$\equiv \ \cdot\ _{L^p}$
$\ \cdot\ _{p_1+p_2}$	$\equiv \ \cdot\ _{L^{p_1+L^{p_2}}}$, where $\ f\ _{L^{p_1+L^{p_2}}} = \inf_{f=f_1+f_2} \ f_1\ _{L^{p_1}} + \ f_2\ _{L^{p_2}}$
$C_c^\infty(\mathbb{R}^d)$	the space of smooth functions with compact support on \mathbb{R}^d
$H^1(\mathbb{R}^d) \equiv H^1$	the Sobolev space of functions on \mathbb{R}^d such that $\ f\ _{H^1} < \infty$, where $\ f\ _{H^1}^2 = \ f\ _2^2 + \ \nabla f\ _2^2$
$H_A^1(\mathbb{R}^d) \equiv H_A^1$	the magnetic Sobolev space of functions on \mathbb{R}^d such that $\ f\ _{H_A^1} < \infty$, where $\ f\ _{H_A^1}^2 = \ f\ _2^2 + \ (-i\nabla + A)f\ _2^2$
$C(I, X)$	the space of continuous functions from I to X , $I \subset \mathbb{R}$ an interval
$L^p(I, X)$	the space of measurable functions $f : I \rightarrow X$ such that $\ f\ _{L^p(I, X)} < \infty$, where $\ f\ _{L^p(I, X)} = \begin{cases} \left(\int_I dt \ f(t)\ _X^p \right)^{\frac{1}{p}} & \text{if } 1 \leq p < \infty, \\ \text{ess sup}_{t \in I} \ f(t)\ _X & \text{if } p = \infty. \end{cases}$

$H^p(I, X)$	the space of functions $f \in L^p(I, X)$ such that $f' \in L^p(I, X)$ in the sense of distributions
$L^q(I, L^r)$	the space of functions $f(t, x) : I \times \mathbb{R}^d \rightarrow \mathbb{C}$, $I \subseteq \mathbb{R}$ an interval, with $\ f\ _{L^q(I, L^r)} = \left(\int_I dt \left(\int_{\mathbb{R}^d} dx f(t, x) ^r \right)^{q/r} \right)^{1/q} < \infty$
$\mathcal{L}(X, Y)$	the space of bounded linear operators from X to Y
$\mathcal{L}(\mathcal{H})$	the space of bounded linear operators on \mathcal{H}
$\mathcal{K}(\mathcal{H})$	the space of compact linear operators on \mathcal{H}
$\mathcal{L}^p(\mathcal{H})$	the p -th trace ideal of $\mathcal{L}(\mathcal{H})$, i.e. the space of operators $A \in \mathcal{L}(\mathcal{H})$ such that $\text{tr} A ^p < \infty$
\mathcal{L}_k	$\equiv \mathcal{L}(\mathcal{H}^{\otimes k})$
\mathcal{L}_k^1	$\equiv \mathcal{L}^1(\mathcal{H}^{\otimes k})$
$\ \cdot\ $	the operator norm on $\mathcal{L}(X, Y)$
$\ \cdot\ _{\mathcal{L}^p}$	the \mathcal{L}^p -norm, $\ \cdot\ _{\mathcal{L}^p} = (\text{tr} \cdot ^p)^{1/p}$
$\text{tr}_{[j_1, \dots, j_l]} \gamma$	the partial trace of a density matrix γ with respect to the particles j_1, \dots, j_l
$[A, B]$	the commutator $AB - BA$
$D(A)$	the domain of an operator A
$\mathcal{Q}(A)$	the form domain of an operator A

Chapter 2

Indicators of convergence

We have introduced the trace norm distance

$$R_N^{(k)}(t) := \operatorname{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right| \quad (2.1)$$

as a meaningful indicator of the closeness $\psi_{N,t} \approx \varphi_t^{\otimes N}$ in (1.9), more precisely as an indicator of the factorisation of $\gamma_{N,t}^{(k)}$ in the limit $N \rightarrow \infty$. However, one can also consider the indicator

$$E_N^{(k)}(t) := 1 - \langle \varphi_t^{\otimes k}, \gamma_{N,t}^{(k)} \varphi_t^{\otimes k} \rangle. \quad (2.2)$$

These two indicators are equivalent in the sense that the vanishing of either one of the two as $N \rightarrow \infty$ implies the vanishing of the other one. However, they differ when considering explicit rates of convergence. In Chapters 4 and 5 we will be working with the indicator $R_N^{(k)}(t)$, while we will be focusing on the indicator $E_N^{(k)}(t)$ in Chapter 6.

In this chapter, we intend to take a closer look at the relationship between the two quantities $R_N^{(k)}(t)$ and $E_N^{(k)}(t)$. The exposition follows largely that of Section 2 in [24]. In addition, we present an improved estimate (2.16).

Let us first consider two examples illustrating the fact that one cannot expect $\psi_{N,t} \approx \varphi_t^{\otimes N}$ to hold in L^2 -norm for large N , but that the convergence of the trace norm distance $\operatorname{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right| \rightarrow 0$ as $N \rightarrow \infty$ is feasible.

Example 2.1. Let $f, g \in L^2(\mathbb{R}^d)$ with $\|f\|_2 = \|g\|_2 = 1$ and define $\psi = f^{\otimes N}$, $\tilde{\psi} = g^{\otimes N}$. Then $\psi, \tilde{\psi} \in L^2(\mathbb{R}^{Nd})$ with $\|\psi\|_2 = \|\tilde{\psi}\|_2 = 1$ and

$$\|\psi - \tilde{\psi}\|_{L^2(\mathbb{R}^{Nd})} = 2 - 2 \operatorname{Re} \langle \psi, \tilde{\psi} \rangle = 2 - 2 \operatorname{Re} (\langle f, g \rangle_{L^2(\mathbb{R}^d)})^N \longrightarrow 2 \quad (2.3)$$

as $N \rightarrow \infty$, if $|\langle f, g \rangle_{L^2(\mathbb{R}^d)}| < 1$. Thus, any two distinct product states become orthogonal in the limit $N \rightarrow \infty$.

Example 2.2. Let $f, g \in L^2(\mathbb{R}^d)$ with $\|f\|_2 = \|g\|_2 = 1$ and $\langle f, g \rangle_{L^2(\mathbb{R}^d)} = 0$. Define $\psi = f^{\otimes N}$ and

$$\tilde{\psi} = \left(f^{\otimes (N-1)} \otimes g \right)_{sym} = \frac{1}{\sqrt{N}} \sum_{j=1}^N f^{(1)} \otimes \dots \otimes f^{(j-1)} \otimes g \otimes f^{(j+1)} \otimes \dots \otimes f^{(N)}. \quad (2.4)$$

Then $\|\psi - \tilde{\psi}\|_2^2 = \|\psi\|_2^2 + \|\tilde{\psi}\|_2^2 = 2$, while we have for the one-particle marginals

$$\gamma_\psi^{(1)} = |f\rangle\langle f|, \quad \gamma_{\tilde{\psi}}^{(1)} = \frac{1}{N}(|g\rangle\langle g| + (N-1)|f\rangle\langle f|) \quad (2.5)$$

and hence,

$$\mathrm{tr} \left| \gamma_\psi^{(1)} - \gamma_{\tilde{\psi}}^{(1)} \right| = \frac{1}{N} \mathrm{tr} \left| (|f\rangle\langle f| - |g\rangle\langle g|) \right| \leq \frac{2}{N} \longrightarrow 0 \quad (2.6)$$

as $N \rightarrow \infty$. Although in this example “only one particle behaves badly”, the L^2 -norm is still too strong. However, the trace norm distance of the two one-particle marginals vanishes in the limit $N \rightarrow \infty$ and thus encodes the appropriate notion of “closeness” between $\gamma_\psi^{(1)}$ and $\gamma_{\tilde{\psi}}^{(1)}$.

In order to investigate the relationship between the two quantities $R_N^{(k)}(t)$ and $E_N^{(k)}(t)$ we consider a more general setup than in the other chapters. Let \mathcal{H} be a Hilbert space with inner product $\langle \cdot, \cdot \rangle$ and induced norm $\|\cdot\|$. We shall use the same notation for the corresponding scalar products and norms on $\mathcal{H}^{\otimes k}$, $k \in \mathbb{N}$. In what follows, \mathcal{L} denotes the space of bounded operators with norm $\|\cdot\|$ and \mathcal{L}^p denotes the p -th trace ideal, $1 \leq p < \infty$, with norm $\|\cdot\|_{\mathcal{L}^p} = (\mathrm{tr} |\cdot|^p)^{1/p}$.

Lemma 2.3. *Let $N \in \mathbb{N}$ and let $\gamma \in \mathcal{L}^1(\mathcal{H}^{\otimes N})$ be a positive trace class operator with unit trace. For $k = 1, \dots, N$, let $\gamma^{(k)} \in \mathcal{L}^1(\mathcal{H}^{\otimes k})$ be the k -particle reduced density matrix associated with γ in the sense of Section 8.1. That is,*

$$\gamma^{(k)} = \mathrm{tr}_{[k+1, \dots, N]} \gamma. \quad (2.7)$$

Let $\varphi \in \mathcal{H}$ satisfy $\|\varphi\| = 1$. For $k = 1, \dots, N$, define

$$E^{(k)} = 1 - \langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \rangle. \quad (2.8)$$

Then we have for $k = 1, \dots, N$

$$E^{(k)} \leq kE^{(1)}. \quad (2.9)$$

Proof. For $k = 1, \dots, N$, let $(\Phi_i^{(k)})_{i \geq 1}$ be an orthonormal basis of $\mathcal{H}^{\otimes k}$ with $\Phi_1^{(k)} = \varphi^{\otimes k}$. By the definition of partial trace as in (8.2), we then have

$$\begin{aligned} \langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \rangle &= \sum_{i \geq 1} \langle \varphi \otimes \Phi_i^{(k-1)}, \gamma^{(k)} \varphi \otimes \Phi_i^{(k-1)} \rangle - \sum_{i \geq 2} \langle \varphi \otimes \Phi_i^{(k-1)}, \gamma^{(k)} \varphi \otimes \Phi_i^{(k-1)} \rangle \\ &= \langle \varphi, \gamma^{(1)} \varphi \rangle - \sum_{i \geq 2} \langle \varphi \otimes \Phi_i^{(k-1)}, \gamma^{(k)} \varphi \otimes \Phi_i^{(k-1)} \rangle. \end{aligned} \quad (2.10)$$

Therefore,

$$\begin{aligned}
& \langle \varphi, \gamma^{(1)} \varphi \rangle - \langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \rangle \\
&= \sum_{i \geq 2} \langle \varphi \otimes \Phi_i^{(k-1)}, \gamma^{(k)} \varphi \otimes \Phi_i^{(k-1)} \rangle \\
&\leq \sum_{i \geq 2} \sum_{j \geq 1} \langle \Phi_j^{(1)} \otimes \Phi_i^{(k-1)}, \gamma^{(k)} \Phi_j^{(1)} \otimes \Phi_i^{(k-1)} \rangle \\
&= \sum_{i \geq 1} \sum_{j \geq 1} \langle \Phi_j^{(1)} \otimes \Phi_i^{(k-1)}, \gamma^{(k)} \Phi_j^{(1)} \otimes \Phi_i^{(k-1)} \rangle - \sum_{j \geq 1} \langle \Phi_j^{(1)} \otimes \varphi^{\otimes(k-1)}, \gamma^{(k)} \Phi_j^{(1)} \otimes \varphi^{\otimes(k-1)} \rangle \\
&= \text{tr } \gamma^{(k)} - \langle \varphi^{\otimes(k-1)}, \gamma^{(k-1)} \varphi^{\otimes(k-1)} \rangle \\
&= 1 - \langle \varphi^{\otimes(k-1)}, \gamma^{(k-1)} \varphi^{\otimes(k-1)} \rangle.
\end{aligned} \tag{2.11}$$

This yields

$$E^{(k)} \leq E^{(k-1)} + E^{(1)}, \tag{2.12}$$

and the claim follows. \square

Remark 2.4. The bound (2.9) is sharp. Indeed, suppose that $E^{(k)} \leq k f(k) E^{(1)}$ for some function f . Then

$$f(k) \geq \sup_{\gamma^{(k)}} \frac{E^{(k)}}{kE^{(1)}} \geq \sup_{0 < \alpha < 1} \frac{1 - (1 - \alpha)^k}{k\alpha} \geq \lim_{\alpha \rightarrow 0} \frac{1 - (1 - \alpha)^k}{k\alpha} = 1, \tag{2.13}$$

where the second inequality follows by restriction of the supremum to product states $\gamma^{(k)} = |\psi\rangle\langle\psi|^{\otimes k}$ and writing $\alpha = E^{(1)}$.

Lemma 2.5. Let $k \in \mathbb{N}$ and let $\gamma^{(k)} \in \mathcal{L}^1(\mathcal{H}^{\otimes k})$ be an arbitrary positive trace class operator with unit trace. Let $\varphi \in \mathcal{H}$ with $\|\varphi\| = 1$. Define

$$E^{(k)} = 1 - \langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \rangle \quad \text{and} \quad R^{(k)} = \|\gamma^{(k)} - |\varphi\rangle\langle\varphi|^{\otimes k}\|_{\mathcal{L}^1}. \tag{2.14}$$

Then

$$E^{(k)} \leq R^{(k)}, \tag{2.15}$$

$$R^{(k)} \leq 2\sqrt{E^{(k)}}. \tag{2.16}$$

Proof. We introduce the shorthand notation

$$p^{(k)} := |\varphi\rangle\langle\varphi|^{\otimes k}. \tag{2.17}$$

Then

$$E^{(k)} = 1 - \langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \rangle = \text{tr}(p^{(k)} - p^{(k)}\gamma^{(k)}) \leq \|p^{(k)}\| \|\gamma^{(k)} - p^{(k)}\|_{\mathcal{L}^1} = R^{(k)}, \tag{2.18}$$

which is (2.15). In order to prove (2.16) we introduce the splitting

$$\begin{aligned}
R^{(k)} &= \|\gamma^{(k)} - p^{(k)}\|_{\mathcal{L}^1} \\
&= \|(p^{(k)} + \mathbb{1} - p^{(k)})\gamma^{(k)} - p^{(k)}\|_{\mathcal{L}^1} \\
&\leq \|p^{(k)}(\gamma^{(k)} - p^{(k)})\|_{\mathcal{L}^1} + \|(\mathbb{1} - p^{(k)})\gamma^{(k)}\|_{\mathcal{L}^1}.
\end{aligned} \tag{2.19}$$

We estimate the first term of (2.19) by

$$\begin{aligned}
\|p^{(k)}(\gamma^{(k)} - p^{(k)})\|_{\mathcal{L}^1} &= \|(p^{(k)})^2(\gamma^{(k)} - p^{(k)})\|_{\mathcal{L}^1} \\
&\leq \|p^{(k)}\|_{\mathcal{L}^2} \|p^{(k)}(\gamma^{(k)} - p^{(k)})\|_{\mathcal{L}^2} \\
&= \left(\langle \varphi^{\otimes k}, (\gamma^{(k)})^2 \varphi^{\otimes k} \rangle - 2 \langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \rangle + 1 \right)^{\frac{1}{2}} \\
&\leq \left(\langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \rangle - 2 \langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \rangle + 1 \right)^{\frac{1}{2}} \\
&= \left(1 - \langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \rangle \right)^{\frac{1}{2}} \\
&= \sqrt{E^{(k)}}.
\end{aligned} \tag{2.20}$$

Now, the second term of (2.19) can be bounded by

$$\begin{aligned}
\|(\mathbf{1} - p^{(k)})\gamma^{(k)}\|_{\mathcal{L}^1} &\leq \|(\mathbf{1} - p^{(k)})\|_{\mathcal{L}^2} \|\gamma^{(k)}\|_{\mathcal{L}^2} \\
&= \left(\text{tr}(\mathbf{1} - p^{(k)}) \right)^{\frac{1}{2}} \\
&= \left(\text{tr}(\mathbf{1} - p^{(k)})\gamma^{(k)} - \text{tr}(\mathbf{1} - p^{(k)})\gamma^{(k)}p^{(k)} \right)^{\frac{1}{2}} \\
&= \left(\text{tr}(\mathbf{1} - p^{(k)})\gamma^{(k)} \right)^{\frac{1}{2}} \\
&= \left(1 - \langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \rangle \right)^{\frac{1}{2}} \\
&= \sqrt{E^{(k)}}.
\end{aligned} \tag{2.21}$$

Note that the first step in (2.21) is just the $\mathcal{L}^1 - \mathcal{L}^2$ Hölder inequality in the form $\|AB\|_{\mathcal{L}^1} \leq \|A\|_{\mathcal{L}^2} \|B\|_{\mathcal{L}^2}$ (see e.g. Chapter 2 in [30] for more details), where $A = \mathbf{1} - p^{(k)}$ and $B = \gamma^{(k)}$. Hence,

$$R^{(k)} \leq 2\sqrt{E^{(k)}}, \tag{2.22}$$

which is (2.16). \square

Remark 2.6. A weaker estimate $R^{(k)} \leq \sqrt{8E^{(k)}}$ is stated in [24]. There the proof is based on the observation that the trace class operator $T := \gamma^{(k)} - p^{(k)}$ can only have one negative eigenvalue, because $\gamma^{(k)}$ is nonnegative and $p^{(k)}$ is a rank-one projection. This was first observed by Seiringer (see Remark 1.4 in [33]).

Then the argument proceeds as follows. Let $(\lambda_n)_{n \geq 0}$ be the sequence of eigenvalues of T and, say, $\lambda_0 \leq 0$. Then $0 = \text{tr} T = \sum_{n=0}^{\infty} \lambda_n$ and therefore

$$\|T\|_{\mathcal{L}^1} = \sum_{n=0}^{\infty} |\lambda_n| = 2|\lambda_0| = 2\|T\| \leq 2\|T\|_{\mathcal{L}^2}. \tag{2.23}$$

Now

$$\|T\|_{\mathcal{L}^2} = \|\gamma^{(k)} - p^{(k)}\|_{\mathcal{L}^2} = \left[\text{tr} \gamma^{(k)} - \text{tr} \gamma^{(k)} p^{(k)} - \text{tr} p^{(k)} \gamma^{(k)} + \text{tr} (p^{(k)})^2 \right]^{1/2} = \sqrt{2E^{(k)}}, \tag{2.24}$$

which yields the result

$$R^{(k)} \leq \sqrt{8E^{(k)}}. \tag{2.25}$$

Remark 2.7. Up to constant factors the bounds (2.15) and (2.16) are sharp, as the following examples show. Consider

$$\varphi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \gamma = \begin{pmatrix} 1-a & 0 \\ 0 & a \end{pmatrix}, \quad (2.26)$$

where $0 \leq a \leq 1$. As above we set $p := |\varphi\rangle\langle\varphi|$. Computation gives

$$E = 1 - \langle\varphi, \gamma\varphi\rangle = a, \quad R = \operatorname{tr} |p - \gamma| = 2a, \quad (2.27)$$

so that (2.15) is sharp up to a constant factor.

In order to show that in general (2.16) is sharp up to a constant factor, consider

$$\varphi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \gamma = \begin{pmatrix} 1-a & \sqrt{a-a^2} \\ \sqrt{a-a^2} & a \end{pmatrix}, \quad (2.28)$$

where $0 \leq a \leq 1$. γ is a density matrix (because it is, in fact, a one-dimensional projector $|\xi\rangle\langle\xi|$, where $\xi = \begin{pmatrix} \sqrt{1-a} \\ \sqrt{a} \end{pmatrix}$). A short calculation yields

$$E = 1 - \langle\varphi, \gamma\varphi\rangle = a \quad (2.29)$$

and

$$\|p\gamma - p\|_{\mathcal{L}^1} = \sqrt{a}. \quad (2.30)$$

Using

$$\|p\gamma - p\|_{\mathcal{L}^1} = \|p(\gamma - p)\|_{\mathcal{L}^1} \leq \|p\| \|\gamma - p\|_{\mathcal{L}^1} \leq \|\gamma - p\|_{\mathcal{L}^1} = R, \quad (2.31)$$

we obtain for this example

$$R \geq \sqrt{E}. \quad (2.32)$$

Chapter 3

The magnetic Hartree equation

An essential step in the derivation of effective evolution equations from quantum dynamics is the passage from a many-body linear Schrödinger equation to an effective description via a one-body nonlinear Schrödinger (NLS) equation. In the analysis presented in the subsequent chapters we need this equation to be globally well-posed.

The local well-posedness of the Hartree equation for suitable interaction potentials was first proven by Ginibre and Velo in [22]. Its global well-posedness then follows from energy methods. Global well-posedness of the magnetic Hartree equation has been established for a constant magnetic field by Cazenave and Esteban in [7]. Salem also treated the well-posedness for a constant magnetic field with smooth, compactly supported perturbations of the magnetic vector field, which are time-dependent, in a web note. NLS equations with more general magnetic field, but with a power-type nonlinearity, have been addressed in [8] and [29].

In this chapter we will give a detailed derivation of the global well-posedness of the magnetic Hartree equation in three dimensions for a slightly more general class of magnetic fields than those considered in [7]. This class includes constant magnetic fields. The idea of the proof is to combine magnetic Strichartz's estimates established by Yajima in [38] with standard techniques for NLS equations (see [6] for a detailed account of these).

For definiteness, we will work in the physically relevant case of three dimensions in this and all subsequent chapters. Most of the results actually hold in any dimension $d \geq 2$, see the concluding remarks in Chapter 7.

The exposition and notation in this chapter is oriented towards that of Cazenave in [6] and we will refer to several results therein. We also refer to the list of symbols in Section 1.6 for some notation.

Let us recall our general assumption on the magnetic vector potential and the generated magnetic field:

Assumption (A). Let $A \in C^\infty(\mathbb{R}^3; \mathbb{R}^3)$ and define $B = \nabla \times A$. Assume that there exists

$\varepsilon > 0$ such that

$$\begin{aligned} |\partial^\alpha B(x)| &\leq C_\alpha (1 + |x|)^{-(1+\varepsilon)} & \forall |\alpha| \geq 1, \forall x \in \mathbb{R}^3, \\ |\partial^\alpha A(x)| &\leq C_\alpha & \forall |\alpha| \geq 1, \forall x \in \mathbb{R}^3, \end{aligned}$$

where C_α are constants depending only on the multi-index α .

Note that the vector potential $A(x) = \frac{1}{2}B_0 \times x$ generating a constant magnetic field B_0 fulfills this assumption. Also, smooth, compactly supported perturbations of linear vector potentials satisfy the hypothesis.

Moreover, the operator $(-i\nabla + A)^2$ can be self-adjointly realised on $L^2(\mathbb{R}^3)$ under the assumption **(A)**. This follows, for instance, from Theorem 2 by Leinfelder and Simader [26].

For $A \in L^2_{loc}(\mathbb{R}^3; \mathbb{R}^3)$ we define the *magnetic Sobolev space* as

$$H^1_A(\mathbb{R}^3) = \{\varphi \in L^2(\mathbb{R}^3) \mid (-i\nabla + A)\varphi \in L^2(\mathbb{R}^3)\}, \quad (3.1)$$

where $\nabla\varphi$ is the distributional gradient of φ . $H^1_A(\mathbb{R}^3)$ is actually a Hilbert space under the inner product

$$\langle \varphi, \psi \rangle_{H^1_A} = \langle \varphi, \psi \rangle + \sum_{j=1}^3 \langle (-i\partial_j + A_j)\varphi, (-i\partial_j + A_j)\psi \rangle. \quad (3.2)$$

We denote by $H^{-1}_A(\mathbb{R}^3)$ the dual space of $H^1_A(\mathbb{R}^3)$.

In the following we consider the initial value problem for the *magnetic Hartree equation*,

$$\begin{cases} i\partial_t \varphi_t = (-i\nabla + A)^2 \varphi_t + (V * |\varphi_t|^2) \varphi_t, \\ \varphi_{t=0} = \varphi. \end{cases} \quad (3.3)$$

The interaction potential $V : \mathbb{R}^3 \rightarrow \mathbb{R}$ will be specified later and the initial data is $\varphi \in H^1_A(\mathbb{R}^3)$. Furthermore, we define the associated energy functional

$$E(\varphi) = \frac{1}{2} \|(-i\nabla + A)\varphi\|_2^2 + \frac{1}{4} \int_{\mathbb{R}^3} (V * |\varphi|^2) |\varphi|^2 \quad \text{for } \varphi \in H^1_A(\mathbb{R}^3). \quad (3.4)$$

Let us define more precisely the notion of a solution to (3.3) and the notion of local and global well-posedness of (3.3).

Definition 3.1. *Let $I \ni 0$ be an interval.*

(i) *A weak H^1_A -solution of (3.3) on I is a function*

$$\varphi_t \in L^\infty(I, H^1_A) \cap H^{1,\infty}(I, H^{-1}_A) \quad (3.5)$$

*such that $i\partial_t \varphi_t = (-i\nabla + A)^2 \varphi_t + (V * |\varphi_t|^2) \varphi_t$ holds in H^{-1}_A for a.a. $t \in I$ and $\varphi_{t=0} = \varphi$.*

(ii) *A strong H^1_A -solution of (3.3) on I is a function*

$$\varphi_t \in C(I, H^1_A) \cap C^1(I, H^{-1}_A) \quad (3.6)$$

*such that $i\partial_t \varphi_t = (-i\nabla + A)^2 \varphi_t + (V * |\varphi_t|^2) \varphi_t$ holds in H^{-1}_A for all $t \in I$ and $\varphi_{t=0} = \varphi$.*

Definition 3.2. We say that the initial-value problem (3.3) is locally well-posed in H_A^1 if the following properties hold:

- (i) For every $\varphi \in H_A^1(\mathbb{R}^3)$ there exists a strong H_A^1 -solution of (3.3) which is defined on a maximal interval $I = (-T_{min}, T_{max})$ with $T_{max} = T_{max}(\varphi) \in (0, \infty]$ and $T_{min} = T_{min}(\varphi) \in (0, \infty]$.
- (ii) There is uniqueness in H_A^1 for the problem (3.3). That is, given any $\varphi \in H_A^1(\mathbb{R}^3)$ and any interval $I \ni 0$, any two weak H_A^1 - solutions of (3.3) on I coincide.
- (iii) There is the blowup alternative: If $T_{max} < \infty$, then $\lim_{t \uparrow T_{max}} \|\varphi_t\|_{H_A^1} = +\infty$ (respectively, if $T_{min} < \infty$, then we have $\lim_{t \downarrow -T_{min}} \|\varphi_t\|_{H_A^1} = +\infty$).
- (iv) The solution depends continuously on the initial value, i.e. if $\varphi_n \xrightarrow{n \rightarrow \infty} \varphi$ in $H_A^1(\mathbb{R}^3)$ and if $I \subset (-T_{min}(\varphi), T_{max}(\varphi))$ is a closed interval, then the maximal solution $\varphi_t^{(n)}$ of (3.3) with the initial condition $\varphi_{t=0}^{(n)} = \varphi_n$ is defined on \bar{I} for n large enough and satisfies $\varphi_t^{(n)} \xrightarrow{n \rightarrow \infty} \varphi_t$ in $C(\bar{I}, H_A^1(\mathbb{R}^3))$.

The problem is globally well-posed if $T_{min} = T_{max} = +\infty$.

We are now in a position to state the main theorem of this chapter.

Theorem 3.3. Let $V(x) = \frac{\lambda}{|x|}$, $\lambda \in \mathbb{R}$, or $V \in L^\infty(\mathbb{R}^3)$ and assume that the vector potential A fulfills assumption **(A)**. Let $\varphi \in H_A^1(\mathbb{R}^3)$. Then the initial value-problem (3.3) is globally well-posed. Moreover there is conservation of mass and energy, i.e.

$$\|\varphi_t\|_2 = \|\varphi\|_2 \quad \text{and} \quad E(\varphi_t) = E(\varphi) \quad \text{for all } t \in \mathbb{R}, \quad (3.7)$$

and $\sup \{ \|\varphi_t\|_{H_A^1} \mid t \in \mathbb{R} \} < \infty$.

The proof of the theorem consists of two steps. We first establish the local well-posedness of (3.3). Using conservation of mass and energy we then show that the solution actually exists globally in time.

3.1 Local well-posedness

We first state the theorem that yields the local well-posedness of (3.3) in $H_A^1(\mathbb{R}^3)$. It follows from an abstract result in [6] on the local well-posedness of NLS-type equations. The main work in this section will be to justify the assumptions of this abstract result. Here, we consider more generally, interaction potentials $V \in L^q(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, $q \geq 1$. In this way we obtain the local well-posedness of (3.3) in $H_A^1(\mathbb{R}^3)$, in particular for the potentials of our interest, $V(x) = \frac{\lambda}{|x|}$, $\lambda \in \mathbb{R}$, and $V \in L^\infty(\mathbb{R}^3)$.

Theorem 3.4. Let $V \equiv V_1 + V_2 \in L^q(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, $q \geq 1$, be real-valued and even with $V_1 \in L^q(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$. Assume that $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ satisfies assumption **(A)** and suppose that the following properties hold:

- (i) $H_A^1(\mathbb{R}^3) \hookrightarrow L^p(\mathbb{R}^3)$ for all $2 \leq p \leq 6$.

(ii) For every $\frac{6}{5} \leq p \leq 6$,

$$(\mathbf{1} + \varepsilon(-i\nabla + A)^2)^{-1} : L^p(\mathbb{R}^3) \rightarrow L^p(\mathbb{R}^3) \quad (3.8)$$

is continuous for all $\varepsilon > 0$, and

$$\sup_{\varepsilon > 0} \left\{ \left\| (\mathbf{1} + \varepsilon(-i\nabla + A)^2)^{-1} \right\|_{\mathcal{L}(L^p; L^p)} \right\} < \infty. \quad (3.9)$$

For $j = 1, 2$ define $g_j(\varphi) := (V_j * |\varphi|^2) \varphi$ for $\varphi \in H_A^1(\mathbb{R}^3)$.

(iii) For $j = 1, 2$, we have $g_j \in C(H_A^1, H_A^{-1})$ such that $g_j = G_j'$ for some $G_j \in C^1(H_A^1, \mathbb{R})$.

(iv) For $j = 1, 2$, there exists $r_j \in [2, 6)$ such that

$$g_j \in C(H_A^1(\mathbb{R}^3), L^{r_j'}(\mathbb{R}^3)) \quad (3.10)$$

and such that for every $M > 0$, there exists $C_j(M) < \infty$ such that

$$\|g_j(\varphi) - g_j(\psi)\|_{L^{r_j'}} \leq C_j(M) \|\varphi - \psi\|_{L^{r_j}} \quad (3.11)$$

for every $\varphi, \psi \in H_A^1$ with $\|\varphi\|_{H_A^1} + \|\psi\|_{H_A^1} \leq M$. Here $\frac{1}{r_j} + \frac{1}{r_j'} = 1$, as usual.

(v) For $j = 1, 2$ and for all $\varphi \in H_A^1(\mathbb{R}^3)$,

$$\operatorname{Im}(g_j(\varphi)\bar{\varphi}) = 0 \text{ a.e. in } \mathbb{R}^3. \quad (3.12)$$

In addition, assume that there is uniqueness for the problem (3.3). Then the initial value problem (3.3) is locally well-posed in $H_A^1(\mathbb{R}^3)$. Moreover, there is conservation of mass and energy, i.e.

$$\|\varphi_t\|_2 = \|\varphi\|_2 \quad \text{and} \quad E(\varphi_t) = E(\varphi) \quad (3.13)$$

for all $t \in (-T_{\min}, T_{\max})$, where φ_t is the solution of (3.3) with initial value $\varphi_{t=0} = \varphi \in H_A^1(\mathbb{R}^3)$.

Proof. Properties (i) - (v) are proven in Lemma 3.5 below. Uniqueness for (3.3) is shown in Proposition 3.8. These are the assumptions of Theorem 3.7.1 in [6], from which the claim follows. \square

In order to prove the assumptions of Theorem 3.4 we will be repeatedly using the following property of the magnetic Sobolev space. It is given in Proposition 8.8 in the appendix. For convenience, let us state it here explicitly for three dimensions.

Proposition 8.8 (Diamagnetic inequality). *Let $A \in L_{loc}^2(\mathbb{R}^3; \mathbb{R}^3)$ and let $\varphi \in H_A^1(\mathbb{R}^3)$. Then $|\varphi| \in H^1(\mathbb{R}^3)$ and the diamagnetic inequality*

$$|\nabla|\varphi|(x)| \leq |(-i\nabla + A)\varphi(x)|$$

holds pointwise for almost every $x \in \mathbb{R}^3$.

Proof. See Theorem 7.21 in [27]. \square

We can now prove the main assumptions of Theorem 3.4 summarised in the next lemma.

Lemma 3.5. *Let $V \equiv V_1 + V_2 \in L^q(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, $q \geq 1$, be real-valued and even. Assume that $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ satisfies the assumption **(A)**. Then the properties (i) - (v) stated as assumptions of Theorem 3.4 hold.*

Proof. (i) From the diamagnetic inequality (8.11) we know that $|\varphi| \in H^1(\mathbb{R}^3)$ for every $\varphi \in H_A^1(\mathbb{R}^3)$. The Sobolev inequality on \mathbb{R}^3 implies that $H^1(\mathbb{R}^3) \hookrightarrow L^6(\mathbb{R}^3)$ and thus $H_A^1(\mathbb{R}^3) \hookrightarrow L^6(\mathbb{R}^3)$. Since $H_A^1(\mathbb{R}^3) \subset L^2(\mathbb{R}^3)$ by definition, we obtain $H_A^1(\mathbb{R}^3) \hookrightarrow L^p(\mathbb{R}^3)$ for all $2 \leq p \leq 6$ by interpolation (8.9).

(ii) The proof of Lemma 9.1.3 in [6] given for a linear magnetic vector potential also works for the more general class of vector potentials satisfying assumption **(A)**.

(iii) and (iv) Set $r_1 = \frac{4q}{2q-1}$ and $r_2 = 2$ as well as $p_1 = q$ and $p_2 = \infty$. Then $r_j \in [2, 6)$ for $j = 1, 2$. Moreover, for $j = 1, 2$, we deduce from Hölder and Young's inequalities that

$$\|(V_j * (uv)) w\|_{L^{r'_j}} \leq \|V_j\|_{L^{p_j}} \|u\|_{L^{r_j}} \|v\|_{L^{r_j}} \|w\|_{L^{r_j}} \quad (3.14)$$

holds for all $u, v, w \in L^{r_j}(\mathbb{R}^3)$. This gives $g_j \in C(L^{r_j}, L^{r'_j})$ and (3.11). Using that $H_A^1(\mathbb{R}^3) \hookrightarrow L^p(\mathbb{R}^3)$ for $2 \leq p \leq 6$ and, by duality, $L^{p'}(\mathbb{R}^3) \hookrightarrow H_A^{-1}(\mathbb{R}^3)$ for $\frac{6}{5} \leq p' \leq 2$, we deduce (3.10) and that $g_j \in C(H_A^1; H_A^{-1})$. For $j = 1, 2$, set

$$G_j(\varphi) = \frac{1}{4} \int_{\mathbb{R}^3} (V_j * |\varphi|^2)(x) |\varphi(x)|^2 dx \quad (3.15)$$

for all measurable $\varphi : \mathbb{R}^3 \rightarrow \mathbb{C}$ such that $(V_j * |\varphi|^2)(x) |\varphi(x)|^2$ is integrable. Again, using $H_A^1(\mathbb{R}^3) \hookrightarrow L^p(\mathbb{R}^3)$ for $2 \leq p \leq 6$ and $L^{p'}(\mathbb{R}^3) \hookrightarrow H_A^{-1}(\mathbb{R}^3)$ for $\frac{6}{5} \leq p' \leq 2$, it then follows as in Proposition 3.2.9 in [6] that $G_j \in C^1(H_A^1, \mathbb{R})$ with $g_j = G'_j$.

(v) This follows from V being real-valued. \square

Finally, we prove the essential assumption of Theorem 3.4, namely that there is uniqueness in H_A^1 for the problem (3.3). To this end we will use magnetic Strichartz's estimates established by Yajima in [38]. For them to hold, the strong assumption **(A)** about the magnetic vector potential is crucial.

Strichartz's estimates are a means to control the size of the solution to the free Schrödinger equation

$$i\partial_t \varphi_t = -\Delta \varphi_t, \quad \varphi_{t=0} = \varphi \in L^2(\mathbb{R}^3) \quad (3.16)$$

in terms of the size of the initial data. It turns out that it is particularly useful to estimate the mixed Lebesgue norms $L^q(I, L^r(\mathbb{R}^3))$, $I \subset \mathbb{R}$ an interval, of the solution $e^{it\Delta} \varphi$ by the $L^2(\mathbb{R}^3)$ -norm of the initial data φ . Since the Schrödinger equation is invariant under the scaling $(t, x) \mapsto (\lambda^2 t, \lambda x)$, these estimates should be invariant under it as well. This leads to the next definition.

Definition 3.6 (Admissible pair). *We say that a pair (q, r) is admissible in three dimensions if*

$$\frac{2}{q} = 3\left(\frac{1}{2} - \frac{1}{r}\right) \quad \text{and} \quad 2 \leq r \leq 6. \quad (3.17)$$

Note that if (q, r) is an admissible pair, then $2 \leq q \leq \infty$.

A large number of such estimates for the free Schrödinger equation (3.16) has been established (see [6] and references therein). Analogous estimates for the free magnetic Schrödinger equation

$$i\partial_t\varphi_t = (-i\nabla + A)^2\varphi_t \quad (3.18)$$

are considerably less known. An important result in this direction was established by Yajima in [38]. It implies the following inhomogeneous magnetic Strichartz's estimate, which we shall need in the rest of the chapter.

Proposition 3.7 (Inhomogeneous magnetic Strichartz's estimate). *Assume that $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ satisfies assumption (A) and define for $t \in \mathbb{R}$ the propagator*

$$\mathcal{T}(t) = e^{-it(-i\nabla+A)^2} : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3). \quad (3.19)$$

Let $0 < |T| < \infty$. If (γ, ρ) is an admissible pair with $\gamma > 2$ and $f \in L^{\gamma'}((0, T), L^{\rho'})$, then for every admissible pair (q, r) with $q > 2$, the function

$$t \mapsto \Phi_f(t) = \int_0^t ds \mathcal{T}(t-s)f(s) \quad (3.20)$$

belongs to $L^q((0, T), L^r)$. Furthermore, there exists a constant C , depending only on γ, ρ and $|T|$, such that

$$\|\Phi_f\|_{L^q((0, T), L^r)} \leq C \|f\|_{L^{\gamma'}((0, T), L^{\rho'})} \quad (3.21)$$

for every $f \in L^{\gamma'}((0, T), L^{\rho'})$. In addition, $\Phi_f \in C([0, T], L^2)$.

Proof. Under the above assumptions, Theorem 4 in [38] by Yajima gives the following explicit representation of the propagator $\mathcal{T}(t)$ as an integral operator for short times t :

There exists $t_0 > 0$ such that for $\psi \in L^2(\mathbb{R}^3)$ and $0 < |t| < t_0$,

$$(\mathcal{T}(t)\psi)(x) = \frac{1}{(2\pi it)^{3/2}} \int_{\mathbb{R}^3} e^{iS(t,x,y)} b(t,x,y) \psi(y) dy, \quad (3.22)$$

where $S(t, x, y)$ is real-valued, C^1 in (t, x, y) , C^∞ in (x, y) for fixed t , and $b(t, x, y)$ is C^1 in (t, x, y) , C^∞ in (x, y) with $|\partial_x^\alpha \partial_y^\beta b(t, x, y)| \leq C_{\alpha\beta}$ for any multi-indices α and β .

Thus, for any $\psi \in L^1(\mathbb{R}^3)$ and $0 < |t| < t_0$, we have

$$\|\mathcal{T}(t)\psi\|_\infty \leq \frac{\|b\|_\infty}{|t|^{3/2}} \|\psi\|_1. \quad (3.23)$$

Hence, there exists a $K > 0$ such that $\mathcal{T}(t)$ maps $L^1(\mathbb{R}^3)$ to $L^\infty(\mathbb{R}^3)$ with a norm less than $K|t|^{-3/2}$ for every $0 < |t| < t_0$.

This last statement is the essential assumption of Theorem 2.7.1 in [6] which yields the claim. \square

With the inhomogeneous magnetic Strichartz's estimate of Proposition 3.7, we can now show uniqueness for the magnetic Hartree equation (3.3).

Proposition 3.8. *Let $\varphi \in H_A^1(\mathbb{R}^3)$ and let $V \equiv V_1 + V_2 \in L^q(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, $q \geq 1$. If $\varphi_t^{(1)}, \varphi_t^{(2)}$ are two weak H_A^1 -solutions of (3.3) with initial data $\varphi \in H_A^1(\mathbb{R}^3)$ on some interval $I \ni 0$ (bounded or unbounded), then $\varphi_t^{(1)} = \varphi_t^{(2)}$.*

Proof. We use the notation $g_j(\varphi) = (V_j * |\varphi|^2)\varphi$ for $j = 1, 2$. Without loss of generality we may assume that I is a bounded interval. By Duhamel's formula (see Proposition 3.1.3 in [6]), φ_t is a weak H_A^1 -solution of (3.3) on an interval $I \ni 0$ if and only if

$$\varphi_t = \mathcal{T}(t)\varphi - i \sum_{j=1}^2 \int_0^t ds \mathcal{T}(t-s) g_j(\varphi_s) \quad \text{for a.a. } t \in I. \quad (3.24)$$

It follows that

$$\varphi_t^{(1)} - \varphi_t^{(2)} = -i \sum_{j=1}^2 \int_0^t ds \mathcal{T}(t-s) (g_j(\varphi_s^{(1)}) - g_j(\varphi_s^{(2)})) \quad \text{for a.a. } t \in I. \quad (3.25)$$

Since $\varphi_t^{(1)}, \varphi_t^{(2)} \in L^\infty(I, H_A^1)$ by assumption, there exists $M > 0$ such that $\|\varphi_t^{(1)}\|_{H_A^1} + \|\varphi_t^{(2)}\|_{H_A^1} \leq M$ for all $t \in I$. Then by property (iv) of Lemma 3.5, for $j = 1, 2$, there exists $r_j \in [2, 6)$ and $C(M) < \infty$ such that for all $t \in I$

$$\|g_j(\varphi_t^{(1)}) - g_j(\varphi_t^{(2)})\|_{L^{r_j'}} \leq C_j(M) \|\varphi_t^{(1)} - \varphi_t^{(2)}\|_{L^{r_j}}. \quad (3.26)$$

For $j = 1, 2$, let now $q_j = \frac{4r_j}{3(r_j-2)}$. Then (q_j, r_j) is an admissible pair and $q_j > 2$. Let J be an arbitrary interval such that $0 \in J \subset I$. For $j = 1, 2$, integration over time yields

$$\|g_j(\varphi_t^{(1)}) - g_j(\varphi_t^{(2)})\|_{L^{q_j'}(J, L^{r_j'})} \leq C_j(M) \|\varphi_t^{(1)} - \varphi_t^{(2)}\|_{L^{q_j'}(J, L^{r_j})}. \quad (3.27)$$

We now apply the magnetic Strichartz's estimates from Proposition 3.7 for the whole interval I . For $j = 1, 2$, we then obtain with $(\gamma, \rho) = (q_j, r_j)$ for $l = 1, 2$ and for every interval $0 \in J \subset I$:

$$\begin{aligned} \left\| \int_0^t ds \mathcal{T}(t-s) (g_j(\varphi_s^{(1)}) - g_j(\varphi_s^{(2)})) \right\|_{L^{q_l}(J, L^{r_l})} &\leq C_j \|g_j(\varphi_t^{(1)}) - g_j(\varphi_t^{(2)})\|_{L^{q_j'}(J, L^{r_j'})} \\ &\leq C_j C_j(M) \|\varphi_t^{(1)} - \varphi_t^{(2)}\|_{L^{q_j'}(J, L^{r_j})}, \end{aligned} \quad (3.28)$$

where we used (3.27) in the second step. Here C_j only depends on q_j, r_j and I , but not on J . Thus, from (3.25) we deduce that for $l = 1, 2$:

$$\begin{aligned} \|\varphi_t^{(1)} - \varphi_t^{(2)}\|_{L^{q_l}(J, L^{r_l})} &\leq \sum_{j=1}^2 \left\| \int_0^t ds \mathcal{T}(t-s) (g_j(\varphi_s^{(1)}) - g_j(\varphi_s^{(2)})) \right\|_{L^{q_l}(J, L^{r_l})} \\ &\leq \sum_{j=1}^2 C_j C_j(M) \|\varphi_t^{(1)} - \varphi_t^{(2)}\|_{L^{q_j'}(J, L^{r_j})}, \end{aligned} \quad (3.29)$$

where we used (3.28) in the second step. Hence, there exists a constant $C > 0$ such that

$$\sum_{j=1}^2 \|\varphi_t^{(1)} - \varphi_t^{(2)}\|_{L^{q_j}(J, L^{r_j})} \leq C \sum_{j=1}^2 \|\varphi_t^{(1)} - \varphi_t^{(2)}\|_{L^{q_j'}(J, L^{r_j})} \quad (3.30)$$

for all intervals J such that $0 \in J \subset I$. The Proposition now follows from applying Lemma 3.9 below with $\phi_j(t) = \|\varphi_t^{(1)} - \varphi_t^{(2)}\|_{L^{r_j}}$, $a_j = q_j'$, $b_j = q_j$ for $j = 1, 2$, since $q_j' < 2 < q_j$ by the choice of (q_j, r_j) . \square

Lemma 3.9. *Let $I \ni 0$ be an interval. Let $1 \leq a_j < b_j \leq \infty$ and $\phi_j \in L^{b_j}(I)$ for $j = 1, 2$. If there exists a constant $C \geq 0$ such that*

$$\sum_{j=1}^2 \|\phi_j\|_{L^{b_j}(J)} \leq C \sum_{j=1}^2 \|\phi_j\|_{L^{a_j}(J)} \quad (3.31)$$

for every interval J with $0 \in J \subset I$, then $\phi_1 = \phi_2 = 0$ a.e. on I .

Proof. This Lemma is a simplified version of Lemma 4.2.2 in [6]. \square

Remark 3.10. The strong assumption **(A)** about the magnetic vector potential A in Theorem 3.3 is needed in order to use Yajima's magnetic Strichartz's estimates to show that there is *a priori* uniqueness for the initial value problem (3.3). Theorem 3.3 could be easily generalised to magnetic vector potentials A satisfying less stringent conditions if magnetic Strichartz's estimates held for these A 's.

Erdoğan, Goldberg and Schlag obtained in [13] magnetic Strichartz's estimates for dimensions $d \geq 3$ for vector potentials A on which they impose significantly weaker regularity conditions than Yajima. However, they require decay of A which excludes linear vector potentials and therefore constant magnetic fields.

Under smallness assumptions about A magnetic Strichartz's estimates for dimensions $d \geq 3$ were obtained by Georgiev, Stefanov and Tarulli in [19]. Their assumptions about A are not satisfied by linear magnetic vector potentials.

Using either of these magnetic Strichartz's estimates should allow one to derive similar global well-posedness results as in Theorem 3.3 for the magnetic Hartree equation under the corresponding assumptions about A . However, these cases have less physical interest, because they do not include the constant magnetic field.

3.2 Global well-posedness

By Theorem 3.4 the magnetic Hartree equation (3.3) is locally well-posed and there is conservation of mass and energy. For $V(x) = \frac{\lambda}{|x|}$, $\lambda \in \mathbb{R}$, we shall now prove that it is globally well-posed. The case $V \in L^\infty(\mathbb{R}^3)$ is easier and therefore omitted.

Proposition 3.11. *Let φ_t be the maximal solution to (3.3) for the interaction potential $V(x) = \frac{\lambda}{|x|}$, $\lambda \in \mathbb{R}$, given by Theorem 3.4. Then φ_t is defined globally in time and there is conservation of mass and energy, i.e.*

$$\|\varphi_t\|_2 = \|\varphi\|_2 \quad \text{and} \quad E(\varphi_t) = E(\varphi) \quad \text{for all } t \in \mathbb{R}. \quad (3.32)$$

Moreover, $\sup \{\|\varphi_t\|_{H_A^1} \mid t \in \mathbb{R}\} < \infty$.

Proof. φ_t is defined on the maximal interval $I = (-T_{min}, T_{max})$ and conservation of mass and energy holds on I . Moreover, by the blowup alternative, if $T_{max} < \infty$, then we have $\lim_{t \uparrow T_{max}} \|\varphi_t\|_{H_A^1} = +\infty$ (respectively, if $T_{min} < \infty$, then we have $\lim_{t \downarrow -T_{min}} \|\varphi_t\|_{H_A^1} = +\infty$). We now control the H_A^1 -norm of φ_t and show that it is uniformly bounded on I . By the blowup alternative, φ_t must then exist globally in time.

For $t \in I$ we have

$$\begin{aligned} E(\varphi_t) &= \frac{1}{2} \|(-i\nabla + A)\varphi_t\|_2^2 + \frac{1}{4} \int_{\mathbb{R}^3} (V * |\varphi_t|^2) |\varphi_t|^2 \\ &\geq \frac{1}{2} \|(-i\nabla + A)\varphi_t\|_2^2 - \frac{|\lambda|}{4} \int_{\mathbb{R}^3} \left| \frac{1}{|\cdot|} * |\varphi_t|^2 \right| |\varphi_t|^2. \end{aligned} \quad (3.33)$$

Using the inequality

$$\frac{1}{|x|} \leq \varepsilon \frac{1}{|x|^2} \mathbf{1}_{\{|x| \leq \varepsilon\}} + \frac{1}{\varepsilon} \mathbf{1}_{\{|x| > \varepsilon\}}, \quad (3.34)$$

which holds for all $\varepsilon > 0$, we can estimate for arbitrary $x \in \mathbb{R}^3$

$$\begin{aligned} \left| \left(\frac{1}{|\cdot|} * |\varphi_t|^2 \right) (x) \right| &= \int_{\mathbb{R}^3} \frac{1}{|x-y|} |\varphi_t(y)|^2 dy \\ &\leq \varepsilon \int_{\mathbb{R}^3} \frac{1}{|x-y|^2} |\varphi_t(y)|^2 dy + \frac{1}{\varepsilon} \int_{\mathbb{R}^3} |\varphi_t(y)|^2 dy \\ &\leq 4\varepsilon \|\nabla_{x-y} |\varphi_t|\|_2^2 + \frac{1}{\varepsilon} \|\varphi_t\|_2^2 \\ &= 4\varepsilon \|\nabla_x |\varphi_t|\|_2^2 + \frac{1}{\varepsilon} \|\varphi_t\|_2^2 \\ &\leq 4\varepsilon \|(-i\nabla_x + A)\varphi_t\|_2^2 + \frac{1}{\varepsilon} \|\varphi_t\|_2^2. \end{aligned} \quad (3.35)$$

Here we used Hardy's inequality (8.10) in the second step, the translational invariance of ∇ in the third step and the diamagnetic inequality (8.11) in the last step.

Using conservation of mass and energy and choosing $\varepsilon = \frac{1}{4|\lambda|\|\varphi\|_2^2}$, yields for all $t \in I$

$$E(\varphi) = E(\varphi_t) \geq \frac{1}{4} \|(-i\nabla + A)\varphi_t\|_2^2 - |\lambda|^2 \|\varphi\|_2^6, \quad (3.36)$$

and hence

$$\|(-i\nabla + A)\varphi_t\|_2^2 \leq 4(E(\varphi) + |\lambda|^2 \|\varphi\|_2^6). \quad (3.37)$$

Thus, we have

$$\|\varphi_t\|_{H_A^1}^2 \leq 4(E(\varphi) + \|\varphi\|_2^2 + |\lambda|^2 \|\varphi\|_2^6) < \infty \quad (3.38)$$

at all times $t \in I$. By the blowup alternative, φ_t exists globally in time. \square

Remark 3.12. The proof of global well-posedness in Proposition 3.11 can be easily adapted to the more general class of interaction potentials $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. For example, all potentials of the type $V(x) = \frac{\lambda}{|x|^\alpha}$, $\lambda \in \mathbb{R}$ and $0 \leq \alpha < 2$, belong to this class. We have local well-posedness of (3.3) for this class of potentials by Theorem 3.4. Let $V \equiv V_1 + V_2$ with $V_1 \in L^{3/2}(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$. It is easy to see that we can decompose V in such a way that $\|V_1\|_{3/2}$ can be made arbitrarily small. We now only show how to perform the analogous estimate to (3.35). Let $x \in \mathbb{R}^3$ be arbitrary. Then

$$\begin{aligned} \left| \left(\frac{1}{|\cdot|} * |\varphi_t|^2 \right) (x) \right| &\leq \int_{\mathbb{R}^3} |V_1(x-y)| |\varphi_t(y)|^2 dy + \|V_2\|_\infty \|\varphi_t\|_2^2 \\ &\leq \|V_1\|_{3/2} \|\varphi_t\|_6^2 + \|V_2\|_\infty \|\varphi_t\|_2^2 \\ &\leq C \|V_1\|_{3/2} \|\nabla |\varphi_t|\|_2^2 + \|V_2\|_\infty \|\varphi_t\|_2^2 \\ &\leq C \|V_1\|_{3/2} \|(-i\nabla + A)\varphi_t\|_2^2 + \|V_2\|_\infty \|\varphi_t\|_2^2. \end{aligned} \quad (3.39)$$

Here we used the Hölder inequality in the second step, the Sobolev inequality in the third step and the diamagnetic inequality (8.11) in the fourth step.

Moreover, we can derive global well-posedness for the potential $V(x) = \frac{\lambda}{|x|^2}$, $\lambda \in \mathbb{R}$, under the smallness condition $|\lambda| < \frac{1}{2\|\varphi\|_2^2}$. To this end, we make use of Hardy's inequality (8.10) in the analogous estimate to (3.35).

Chapter 4

Perturbative expansion of the BBGKY hierarchy

In this chapter we will prove that for bounded potentials the limiting quantum dynamics for mean-field systems with magnetic fields in three dimensions is determined by the solution to the magnetic Hartree equation (3.3). We will apply a method first developed by Spohn in [37] for non-relativistic mean-field systems, which is based on a perturbative expansion of the so-called BBGKY hierarchy. We will largely follow the exposition of [35] for the description of Spohn's approach. Along the way we will present the minor changes needed to extend this method in order to include magnetic fields. The main result of this chapter is as follows.

Theorem 4.1. *Let $V \in L^\infty(\mathbb{R}^3)$ and assume that the magnetic vector potential $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ satisfies assumption (A). We consider the mean-field quantum dynamics generated by the Hamiltonian*

$$H_N = \sum_{j=1}^N h_j + \frac{1}{N} \sum_{i < j}^N V(x_i - x_j), \quad (4.1)$$

where $h = (-i\nabla + A)^2$ is the magnetic one-particle operator. Let $\varphi \in H_A^1(\mathbb{R}^3)$ with $\|\varphi\|_2 = 1$ and set $\psi_N = \varphi^{\otimes N}$. Let $\psi_{N,t} = e^{-iH_N t} \psi_N$ and denote by φ_t the solution to the magnetic Hartree equation (3.3) with initial data $\varphi_{t=0} = \varphi$. Denote by $\gamma_{N,t}^{(k)}$ the k -particle marginals associated with $\psi_{N,t}$. Then, for every fixed $k \in \mathbb{N}$ and for every fixed $t \in \mathbb{R}$, we have

$$\lim_{N \rightarrow \infty} \operatorname{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle \langle \varphi_t|^{\otimes k} \right| = 0. \quad (4.2)$$

Before we can embark on the proof of Theorem 4.1, we have to introduce the BBGKY hierarchy, the main tool of this and the next chapter. We know that the state of a mean-field quantum system of N identical bosons is given by a symmetric and normalised wave function $\psi_{N,t} \in L^2(\mathbb{R}^{Nd})$ whose evolution is governed by the Schrödinger equation (1.4). Equivalently, we can consider the density matrix $\gamma_{N,t} = |\psi_{N,t}\rangle \langle \psi_{N,t}|$, whose time evolution is determined by the von Neumann equation

$$\begin{cases} i\partial_t \gamma_{N,t} = [H_N, \gamma_{N,t}], \\ \gamma_{N,t=0} = \gamma_N. \end{cases} \quad (4.3)$$

The description of the dynamics of the system in terms of the wave function $\psi_{N,t}$ and the Schrödinger equation is equivalent to the description in terms of the density matrix $\gamma_{N,t}$ and

the von Neumann equation.

Owing to the interactions between the particles, the dynamics of the k -particle marginal $\gamma_{N,t}^{(k)}$ cannot be described by a closed equation in $\gamma_{N,t}^{(k)}$. The correct evolution law for $\gamma_{N,t}^{(k)}$ is obtained by taking the partial trace over $(N - k)$ particles in the von Neumann equation and by exploiting the boson symmetry of the marginals. The result is a hierarchy of coupled evolution equations for $k = 1, \dots, N$:

$$\begin{cases} i\partial_t \gamma_{N,t}^{(k)} = \sum_{j=1}^k [h_j, \gamma_{N,t}^{(k)}] + \frac{1}{N} \sum_{i<j}^k [V(x_i - x_j), \gamma_{N,t}^{(k)}] + \frac{N-k}{N} \sum_{j=1}^k \text{tr}_{[k+1]} [V(x_j - x_{k+1}), \gamma_{N,t}^{(k+1)}], \\ \gamma_{N,t=0}^{(k)} = \gamma_N^{(k)}. \end{cases} \quad (4.4)$$

Here $\text{tr}_{[k+1]}$ denotes the partial trace over the $(k+1)$ -th particle and we use the convention that $\gamma_{N,t}^{(k)} = 0$ if $k > N$. (4.4) is the celebrated BBGKY hierarchy named after the mathematicians and physicists Bogoliubov, Born, Green, Kirkwood and Yvon. Its structure is such that the time derivative of the k -th marginal is expressed in terms of the k -th marginal *and* the $(k+1)$ -th marginal. Notice that choosing $k = N$ just gives the von Neumann equation, so that the introduction of the hierarchy of equations might look tautological. But we will see in this and the next chapter that the BBGKY hierarchy is an appropriate tool for considering the limiting dynamics as $N \rightarrow \infty$.

Taking the *formal* limit $N \rightarrow \infty$ in (4.4) leads to an infinite hierarchy of coupled equations for a family of marginal densities $\{\gamma_{\infty,t}^{(k)}\}_{k \in \mathbb{N}}$:

$$\begin{cases} i\partial_t \gamma_{\infty,t}^{(k)} = \sum_{j=1}^k [h_j, \gamma_{\infty,t}^{(k)}] + \sum_{j=1}^k \text{tr}_{[k+1]} [V(x_j - x_{k+1}), \gamma_{\infty,t}^{(k+1)}], \\ \gamma_{\infty,t=0}^{(k)} = \gamma_{\infty,0}^{(k)}, \end{cases} \quad (4.5)$$

where $\{\gamma_{\infty,0}^{(k)}\}_{k \in \mathbb{N}}$ is the family of initial states.

Proof of Theorem 4.1. By Duhamel's formula we can rewrite each equation of the hierarchy (4.4) in integral form as

$$\gamma_{N,t}^{(k)} = \mathcal{U}^{(k)}(t) \gamma_N^{(k)} + \frac{1}{N} \int_0^t ds \mathcal{U}^{(k)}(t-s) A^{(k)} \gamma_{N,s}^{(k)} + \frac{N-k}{N} \int_0^t ds \mathcal{U}^{(k)}(t-s) B^{(k)} \gamma_{N,s}^{(k+1)}, \quad (4.6)$$

where we defined the free evolution operator

$$\mathcal{U}^{(k)}(t) \gamma^{(k)} := e^{-it \sum_{j=1}^k h_j} \gamma^{(k)} e^{it \sum_{j=1}^k h_j}, \quad (4.7)$$

and the operators

$$A^{(k)} \gamma^{(k)} = -i \sum_{i<j}^k [V(x_i - x_j), \gamma^{(k)}], \quad (4.8)$$

$$B^{(k)} \gamma^{(k+1)} = -i \sum_{j=1}^k \text{tr}_{[k+1]} [V(x_j - x_{k+1}), \gamma^{(k+1)}]. \quad (4.9)$$

The free evolution operator $\mathcal{U}^{(k)}(t)$ is well-defined, because the one-particle operator h is self-adjoint under the assumptions on the magnetic vector potential A (see e.g. Theorem 2 in [26]). Also, notice that $A^{(k)}$ maps k -particle operators into k -particle operators, while $B^{(k)}$ maps $(k+1)$ -particle operators into k -particle operators.

The infinite hierarchy (4.5) in integral form is given by the equations

$$\gamma_{\infty,t}^{(k)} = \mathcal{U}^{(k)}(t)\gamma_{\infty,0}^{(k)} + \int_0^t ds \mathcal{U}^{(k)}(t-s)B^{(k)}\gamma_{\infty,s}^{(k+1)} \quad (4.10)$$

for every $k \in \mathbb{N}$ and with initial data $\{\gamma_{\infty,0}^{(k)}\}_{k \in \mathbb{N}} = \{|\varphi\rangle\langle\varphi|^{\otimes k}\}_{k \in \mathbb{N}}$. One sees by direct inspection that the family $\{|\varphi_t\rangle\langle\varphi_t|^{\otimes k}\}_{k \in \mathbb{N}}$ is a solution to the infinite hierarchy, where φ_t is the solution to the magnetic Hartree equation (3.3) with initial data $\varphi_{t=0} = \varphi$. We will actually see in the third part of the proof of Theorem 5.1 that this family is the unique solution.

In order to estimate the trace norm distance $\text{tr} \left| \gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)} \right| \equiv \|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1}$, we iterate the integral expressions for $\gamma_{N,t}^{(k)}$ and $\gamma_{\infty,t}^{(k)}$. Since we are interested in the limit $N \rightarrow \infty$ for fixed $k \in \mathbb{N}$, we understand the second term on the right-hand side of (4.6) as well as the contribution proportional to $\frac{k}{N}$ to the third term on the right-hand side of (4.6) as small perturbations. Iterating the integral equation (4.6) n times, and stopping the iteration every time we encounter a perturbation, we obtain

$$\begin{aligned} \gamma_{N,t}^{(k)} &= \mathcal{U}^{(k)}(t)\gamma_N^{(k)} \\ &+ \sum_{m=1}^{n-1} \int_0^t ds_1 \cdots \int_0^{s_{m-1}} ds_m \mathcal{U}^{(k)}(t-s_1)B^{(k)}\mathcal{U}^{(k+1)}(s_1-s_2) \cdots B^{(k+m-1)}\mathcal{U}^{(k+m)}(s_m)\gamma_N^{(k+m)} \\ &+ \int_0^t ds_1 \cdots \int_0^{s_{n-1}} ds_n \mathcal{U}^{(k)}(t-s_1)B^{(k)}\mathcal{U}^{(k+1)}(s_1-s_2) \cdots B^{(k+n-1)}\gamma_{N,s_n}^{(k+n)} \\ &+ \frac{1}{N} \sum_{m=1}^n \int_0^t ds_1 \cdots \int_0^{s_{m-1}} ds_m \mathcal{U}^{(k)}(t-s_1)B^{(k)} \cdots \mathcal{U}^{(k+m-1)}(s_{m-1}-s_m)A^{(k+m-1)}\gamma_{N,s_m}^{(k+m-1)} \\ &- \sum_{m=1}^n \frac{k+m-1}{N} \int_0^t ds_1 \cdots \int_0^{s_{m-1}} ds_m \mathcal{U}^{(k)}(t-s_1)B^{(k)} \cdots B^{(k+m-1)}\gamma_{N,s_m}^{(k+m)}. \end{aligned} \quad (4.11)$$

Iterating the infinite hierarchy in integral form (4.10) for n times yields

$$\begin{aligned} \gamma_{\infty,t}^{(k)} &= \mathcal{U}^{(k)}(t)\gamma_{\infty,0}^{(k)} \\ &+ \sum_{m=1}^{n-1} \int_0^t ds_1 \cdots \int_0^{s_{m-1}} ds_m \mathcal{U}^{(k)}(t-s_1)B^{(k)}\mathcal{U}^{(k+1)}(s_1-s_2) \cdots B^{(k+m-1)}\mathcal{U}^{(k+m)}(s_m)\gamma_{\infty,0}^{(k+m)} \\ &+ \int_0^t ds_1 \cdots \int_0^{s_{n-1}} ds_n \mathcal{U}^{(k)}(t-s_1)B^{(k)}\mathcal{U}^{(k+1)}(s_1-s_2) \cdots B^{(k+n-1)}\gamma_{\infty,s_n}^{(k+n)}. \end{aligned} \quad (4.12)$$

Using that $\gamma_{\infty,0}^{(k)} = \gamma_N^{(k)} = |\varphi\rangle\langle\varphi|^{\otimes k}$ for all $k \in \mathbb{N}$, we begin to estimate the difference

$$\begin{aligned}
& \|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} \\
& \leq \int_0^t ds_1 \cdots \int_0^{s_{n-1}} ds_n \|\mathcal{U}^{(k)}(t-s_1)B^{(k)}\mathcal{U}^{(k+1)}(s_1-s_2) \cdots B^{(k+n-1)}(\gamma_{N,s_n}^{(k+n)} - \gamma_{\infty,s_n}^{(k+n)})\|_{\mathcal{L}^1} \\
& \quad + \frac{1}{N} \sum_{m=1}^n \int_0^t ds_1 \cdots \int_0^{s_{m-1}} ds_m \|\mathcal{U}^{(k)}(t-s_1)B^{(k)} \cdots \mathcal{U}^{(k+m-1)}(s_{m-1}-s_m)A^{(k+m-1)}\gamma_{N,s_m}^{(k+m-1)}\|_{\mathcal{L}^1} \\
& \quad + \sum_{m=1}^n \frac{k+m-1}{N} \int_0^t ds_1 \cdots \int_0^{s_{m-1}} ds_m \|\mathcal{U}^{(k)}(t-s_1)B^{(k)} \cdots B^{(k+m-1)}\gamma_{N,s_m}^{(k+m)}\|_{\mathcal{L}^1}.
\end{aligned} \tag{4.13}$$

To proceed with the estimate we use the fact that the volume of the n -simplex with side length t is given by $\int_0^t ds_1 \cdots \int_0^{s_{n-1}} ds_n 1 = \frac{t^n}{n!}$ and we use the following bounds. By the unitarity of the free evolution $\mathcal{U}^{(k)}(t)$ we have

$$\|\mathcal{U}^{(k)}(t)\gamma^{(k)}\|_{\mathcal{L}^1} = \text{tr} \left| \mathcal{U}^{(k)}(t)\gamma^{(k)} \right| = \text{tr} \left| \gamma^{(k)} \right| = \|\gamma^{(k)}\|_{\mathcal{L}^1}. \tag{4.14}$$

Since V is bounded, we have additionally

$$\|A^{(k)}\gamma^{(k)}\|_{\mathcal{L}^1} \leq k^2 \|V\| \|\gamma^{(k)}\|_{\mathcal{L}^1} \tag{4.15}$$

and

$$\|B^{(k)}\gamma^{(k+1)}\|_{\mathcal{L}^1} \leq 2k \|V\| \|\gamma^{(k)}\|_{\mathcal{L}^1}, \tag{4.16}$$

where we used the fact (see (8.6)) that

$$\text{tr} \left| \text{tr}_{[k+1]} \gamma^{(k+1)} \right| \leq \text{tr} \left| \gamma^{(k+1)} \right|. \tag{4.17}$$

We iteratively apply the bounds (4.14), (4.15) and (4.16) to the terms on the right-hand side of (4.13) and finally use the trivial bounds $\|\gamma_{N,t}^{(k)}\|_{\mathcal{L}^1} = \|\gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} = 1$ as well as $\|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} \leq 2$, which hold for all $k \in \mathbb{N}$, to obtain

$$\|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} \leq 2(2\|V\|t)^n \frac{(k+n-1)!}{(k-1)!n!} + \frac{2}{N} \sum_{m=1}^n (2\|V\|t)^m (k+m-1) \frac{(k+m-1)!}{(k-1)!m!}. \tag{4.18}$$

Next we observe that

$$\frac{(k+n-1)!}{(k-1)!n!} = \binom{k+n-1}{n} \leq \sum_{l=0}^{k+n-1} \binom{k+n-1}{l} = 2^{k+n-1} \tag{4.19}$$

and

$$(k+m-1) \frac{(k+m-1)!}{m!(k-1)!} = k \binom{k+m-1}{k-1} + \frac{m-1}{m} k \binom{k+m-1}{k} \leq 2k 2^{k+m-1}. \tag{4.20}$$

Hence,

$$\|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} \leq 2^k (4\|V\|t)^n + \frac{k2^{k+1}}{N} \sum_{m=1}^n (4\|V\|t)^m. \tag{4.21}$$

We will first prove the convergence $\|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} \rightarrow 0$ as $N \rightarrow \infty$ for short times and then deduce by a contradiction argument that it actually holds at all times. So if $0 < t \leq t_0$, where $t_0 = \frac{1}{8\|V\|}$, then

$$\|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} \leq \frac{2^k}{2^n} + \frac{k2^{k+1}}{N}. \quad (4.22)$$

Since the left-hand side of (4.22) is independent of n , it follows that

$$\|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} \leq \frac{k2^{k+1}}{N}. \quad (4.23)$$

Thus,

$$\lim_{N \rightarrow \infty} \|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} = 0 \quad (4.24)$$

for all fixed $0 \leq t \leq t_0$ and for all fixed $k \in \mathbb{N}$.

Next we define

$$t_1 := \sup \left\{ t > 0 \mid \lim_{N \rightarrow \infty} \|\gamma_{N,s}^{(k)} - \gamma_{\infty,s}^{(k)}\|_{\mathcal{L}^1} = 0 \text{ for all fixed } 0 \leq s \leq t \text{ and all fixed } k \in \mathbb{N} \right\}. \quad (4.25)$$

From (4.24) we know that $t_1 \geq t_0$. By contradiction we show that actually $t_1 = \infty$.

Suppose that $t_1 < \infty$. For $t_2 = t_1 - \frac{t_0}{2}$, we have, by the definition of t_1 , that for fixed $k \in \mathbb{N}$,

$$\lim_{N \rightarrow \infty} \|\gamma_{N,t_2}^{(k)} - \gamma_{\infty,t_2}^{(k)}\|_{\mathcal{L}^1} = 0 \quad (4.26)$$

holds. Starting from this, we will show that for every fixed $k \in \mathbb{N}$

$$\lim_{N \rightarrow \infty} \|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} = 0 \quad (4.27)$$

actually holds for all $0 < t \leq t_1 + \frac{t_0}{2}$, which will contradict the definition of t_1 .

To this end we expand the integral expressions for $\gamma_{N,t}^{(k)}$ and $\gamma_{\infty,t}^{(k)}$ in a similar manner as before, but starting at time t_2 . This yields for time $t = t_2 + \tau$, $0 \leq \tau \leq t_0$,

$$\begin{aligned} & \|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} \\ \leq & \|\mathcal{U}^{(k)}(\tau)(\gamma_{N,t_2}^{(k)} - \gamma_{\infty,t_2}^{(k)})\|_{\mathcal{L}^1} \\ & + \sum_{m=1}^{n-1} \int_0^\tau ds_1 \cdots \int_0^{s_{m-1}} ds_m \times \\ & \quad \|\mathcal{U}^{(k)}(\tau - s_1)B^{(k)}\mathcal{U}^{(k+1)}(s_1 - s_2) \cdots B^{(k+m-1)}\mathcal{U}^{(k+m)}(s_m)(\gamma_{N,t_2}^{(k+m)} - \gamma_{\infty,t_2}^{(k+m)})\|_{\mathcal{L}^1} \\ & + \int_0^\tau ds_1 \cdots \int_0^{s_{n-1}} ds_n \|\mathcal{U}^{(k)}(\tau - s_1)B^{(k)}\mathcal{U}^{(k+1)}(s_1 - s_2) \cdots B^{(k+n-1)}(\gamma_{N,t_2+s_n}^{(k+n)} - \gamma_{\infty,t_2+s_n}^{(k+n)})\|_{\mathcal{L}^1} \\ & + \frac{1}{N} \sum_{m=1}^n \int_0^\tau ds_1 \cdots \int_0^{s_{m-1}} ds_m \|\mathcal{U}^{(k)}(\tau - s_1)B^{(k)} \cdots \mathcal{U}^{(k+m-1)}(s_{m-1} - s_m)A^{(k+m-1)}\gamma_{N,t_2+s_m}^{(k+m-1)}\|_{\mathcal{L}^1} \\ & + \sum_{m=1}^n \frac{k+m-1}{N} \int_0^\tau ds_1 \cdots \int_0^{s_{m-1}} ds_m \|\mathcal{U}^{(k)}(\tau - s_1)B^{(k)} \cdots B^{(k+m-1)}\gamma_{N,t_2+s_m}^{(k+m)}\|_{\mathcal{L}^1}. \end{aligned} \quad (4.28)$$

More terms appear in this estimate than in (4.13), because the k -particle marginals $\gamma_{N,t_2}^{(k)}$ and $\gamma_{\infty,t_2}^{(k)}$, $k \in \mathbb{N}$, do not necessarily coincide at time $t_2 > 0$. Proceeding in an analogous way as before using the estimates (4.14), (4.15), (4.16) and the trivial estimates $\|\gamma_{N,t}^{(k)}\|_{\mathcal{L}^1} = \|\gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} = 1$ as well as $\|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} \leq 2$, which hold for all $k \in \mathbb{N}$, we obtain

$$\|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} \leq 2^k \sum_{m=0}^{n-1} \frac{1}{2^m} \|\gamma_{N,t_2}^{(k+m)} - \gamma_{\infty,t_2}^{(k+m)}\|_{\mathcal{L}^1} + \frac{2^k}{2^n} + \frac{k2^{k+1}}{N}. \quad (4.29)$$

Now let $\varepsilon > 0$ be arbitrary. First choose n large enough such that $\frac{2^k}{2^n} \leq \frac{\varepsilon}{3}$. Then choose N large enough such that the first and third term are each less than $\frac{\varepsilon}{3}$. This is possible because, by assumption, for time $t_2 < t_1$ we have $\|\gamma_{N,t_2}^{(k+m)} - \gamma_{\infty,t_2}^{(k+m)}\|_{\mathcal{L}^1} \rightarrow 0$ as $N \rightarrow \infty$. Since $\varepsilon > 0$ was chosen arbitrarily, this implies

$$\lim_{N \rightarrow \infty} \|\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)}\|_{\mathcal{L}^1} = 0 \quad (4.30)$$

for $t_1 - \frac{t_0}{2} \leq t \leq t_1 + \frac{t_0}{2}$, which completes the proof. \square

Remark 4.2. Let us emphasise that in order to include an external magnetic field by Spohn's method a minor change and a non-trivial part are both needed. One has to use the free evolution operator $\mathcal{U}^{(k)}(t)$ acting on k -particle marginals $\gamma^{(k)}$ by

$$\mathcal{U}^{(k)}(t)\gamma^{(k)} = e^{-it \sum_{j=1}^k (-i\nabla_j + A(x_j))^2} \gamma^{(k)} e^{it \sum_{j=1}^k (-i\nabla_j + A(x_j))^2} \quad (4.31)$$

instead of the free evolution operator

$$\tilde{\mathcal{U}}^{(k)}(t)\gamma^{(k)} = e^{it \sum_{j=1}^k \Delta_j} \gamma^{(k)} e^{-it \sum_{j=1}^k \Delta_j} \quad (4.32)$$

for non-relativistic systems without magnetic fields. $\mathcal{U}^{(k)}(t)$ is well-defined because the operator $(-i\nabla + A)^2$ is self-adjoint under the assumptions **(A)** on the magnetic vector potential A . What is instead non-trivial in generalising Spohn's method to Theorem 4.1 is the fact that the magnetic Hartree equation is globally well-posed in $H_A^1(\mathbb{R}^3)$. This was shown in Chapter 3.

In [11], Erdős and Schlein used a new approach inspired by Lieb-Robinson bounds to obtain estimates of the rate of convergence under more restrictive conditions applying to the interaction potential V . Their method is also based on the BBGKY hierarchy and it can be easily generalised to non-relativistic mean-field quantum systems with magnetic fields. Similar to the proof of Theorem 4.1 one also only has to use a different free evolution operator. This gives the next result.

Theorem 4.3. *Let $V \in L^\infty(\mathbb{R}^3)$ such that $\|\widehat{V}\|_1 < \infty$ and assume that the magnetic vector potential $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ satisfies assumption **(A)**. We consider the mean-field quantum dynamics generated by the Hamiltonian*

$$H_N = \sum_{j=1}^N h_j + \frac{1}{N} \sum_{i < j}^N V(x_i - x_j), \quad (4.33)$$

where $h = (-i\nabla + A)^2$ is the magnetic one-particle operator. Let $\varphi \in H_A^1(\mathbb{R}^3)$ with $\|\varphi\|_2 = 1$ and set $\psi_N = \varphi^{\otimes N}$. Let $\psi_{N,t} = e^{-iH_N t} \psi_N$ and denote by φ_t the solution to the magnetic Hartree equation (3.3) with initial data $\varphi_{t=0} = \varphi$. Denote by $\gamma_{N,t}^{(k)}$ the k -particle marginals associated with $\psi_{N,t}$. Then we have

$$\mathrm{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right| \leq \frac{k^2 \lambda_V}{N} e^{2k\|V\|_\infty} \left(e^{8\|V\|_\infty t} - 1 \right) \quad (4.34)$$

for every $t \in \mathbb{R}$, $N \geq 1$ and $1 \leq k \leq N$. Here $\lambda_V = 1 + (\|\widehat{V}\|_1 / \|V\|_\infty)$.

Proof. The proof is a straightforward generalisation of the proof in [11] by using the magnetic free evolution operator (4.31) instead of (4.32) for non-relativistic systems without magnetic fields. Apart from the global well-posedness of (3.3), the self-adjointness of $(-i\nabla + A)^2$ is again all that is needed. This holds under the assumption **(A)**. \square

Chapter 5

A compactness argument based on the BBGKY hierarchy

In [2], [3] and [12], Bardos, Erdős, Golse, Mauser and Yau developed an alternative approach to mean-field quantum dynamics, which is also based on the BBGKY hierarchy. Their method relies on a compactness argument and in this way avoids the expansion of the BBGKY hierarchy.

In this chapter we will use their method to include an external magnetic field. The description of the method mainly follows that of [35] and Sections 6 and 7 in [14]. Along the way, we will discuss in detail those steps of the original proof that we managed to modify and adapt for the inclusion of an external magnetic field.

We assume that the interaction potential V is bounded and that it vanishes at infinity, i.e. $V(x) \rightarrow 0$ as $|x| \rightarrow \infty$. This additional assumption is justified in the sense that all physically reasonable potentials vanish at infinity. The main result is as follows.

Theorem 5.1. *Let $V \in L^\infty(\mathbb{R}^3)$ such that $V(x) \rightarrow 0$ as $|x| \rightarrow \infty$ and assume that the magnetic vector potential $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ satisfies assumption **(A)**. We consider the mean-field quantum dynamics generated by the Hamiltonian*

$$H_N = \sum_{j=1}^N h_j + \frac{1}{N} \sum_{i < j}^N V(x_i - x_j), \quad (5.1)$$

where $h = (-i\nabla + A)^2$ is the magnetic one-particle operator. Let $\varphi \in H_A^1(\mathbb{R}^3)$ with $\|\varphi\|_2 = 1$ and set $\psi_N = \varphi^{\otimes N}$. Let $\psi_{N,t} = e^{-iH_N t} \psi_N$ and denote by φ_t the solution to the magnetic Hartree equation (3.3) with initial data $\varphi_{t=0} = \varphi$. Denote by $\gamma_{N,t}^{(k)}$ the k -particle marginals associated with $\psi_{N,t}$. Then, for every fixed $k \in \mathbb{N}$ and for every fixed $t \in \mathbb{R}$, we have

$$\lim_{N \rightarrow \infty} \operatorname{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle \langle \varphi_t|^{\otimes k} \right| = 0. \quad (5.2)$$

Proof. For every $N \in \mathbb{N}$, we denote by $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ the family of k -particle marginals associated with the wavefunction $\psi_{N,t}$. The evolution equations for the elements of $\Gamma_{N,t}$ are

given by the BBGKY hierarchy of equations (4.4). In what follows, we consider the infinite hierarchy with initial data $\{|\varphi\rangle\langle\varphi|^{\otimes k}\}_{k\in\mathbb{N}}$ for a family of marginal densities $\{\gamma_{\infty,t}^{(k)}\}_{k\in\mathbb{N}}$:

$$\begin{cases} i\partial_t\gamma_{\infty,t}^{(k)} = \sum_{j=1}^k [h_j, \gamma_{\infty,t}^{(k)}] + \sum_{j=1}^k \text{tr}_{[k+1]} [V(x_j - x_{k+1}), \gamma_{\infty,t}^{(k+1)}], \\ \gamma_{\infty,t=0}^{(k)} = |\varphi\rangle\langle\varphi|^{\otimes k}. \end{cases} \quad (5.3)$$

The main idea of the proof is to characterise the limit of the sequence $(\Gamma_{N,t})_{N\in\mathbb{N}}$ as the unique solution to the infinite hierarchy of equations (5.3). The proof consists of three steps. We first show the precompactness of the sequence $(\Gamma_{N,t})_{N\in\mathbb{N}}$ with respect to an appropriate weak topology. Next we identify each limit point of the sequence $(\Gamma_{N,t})_{N\in\mathbb{N}}$ as a solution to the infinite hierarchy of equations (5.3). Finally, we prove the uniqueness of the solution to the infinite hierarchy (5.3).

One sees by direct inspection that the family $\{\gamma_{\infty,t}^{(k)}\}_{k\in\mathbb{N}}$ with $\gamma_{\infty,t}^{(k)} = |\varphi_t\rangle\langle\varphi_t|^{\otimes k}$ solves the infinite hierarchy (5.3). Since a precompact sequence with only one limit point actually converges to this point, it follows for every $k\in\mathbb{N}$ that $\gamma_{N,t}^{(k)} \rightarrow |\varphi_t\rangle\langle\varphi_t|^{\otimes k}$ as $N \rightarrow \infty$ in the weak operator topology. Using the fact that the limit point is an orthogonal rank one projection, we then show that this convergence also holds in trace norm. We now explain in detail the three steps of the proof.

Step 1: Precompactness

Let $\mathcal{L}_k^1 \equiv \mathcal{L}^1(L^2(\mathbb{R}^{3k}))$ denote the space of trace class operators on $L^2(\mathbb{R}^{3k})$ equipped with the trace norm $\|\cdot\|_{\mathcal{L}^1}$. Moreover, let $\mathcal{K}_k \equiv \mathcal{K}(L^2(\mathbb{R}^{3k}))$ be the space of compact operators on $L^2(\mathbb{R}^{3k})$ equipped with the operator norm $\|\cdot\|$. Then \mathcal{L}_k^1 and \mathcal{K}_k are Banach spaces and $\mathcal{L}_k^1 = \mathcal{K}_k^*$ (see e.g. Theorem VI.26 in [32]).

By definition, the k -particle marginals $\gamma_{N,t}^{(k)}$ are nonnegative trace class operators with unit trace:

$$\|\gamma_{N,t}^{(k)}\|_{\mathcal{L}^1} = \text{tr} |\gamma_{N,t}^{(k)}| = \text{tr} \gamma_{N,t}^{(k)} = 1. \quad (5.4)$$

For fixed $t\in\mathbb{R}$ and fixed $k\in\mathbb{N}$, it follows from the Banach-Alaoglu Theorem that $\{\gamma_{N,t}^{(k)}\}_{N\geq k}$ has a weak* - convergent subsequence in \mathcal{L}_k^1 .

However, precompactness at fixed times $t\in\mathbb{R}$ is not enough. We need the precompactness of the sequence $(\Gamma_{N,t})_{N\in\mathbb{N}}$ uniformly on an entire time interval in order to be able to show that a limit point of the sequence is a solution to the infinite hierarchy of equations (5.3). This leads to the definition of the appropriate weak topology. To this end we use the fact that the weak* topology on the unit ball of \mathcal{L}_k^1 is metrisable, because its predual \mathcal{K}_k is separable. We fix a dense countable subset of the unit ball of \mathcal{K}_k , say $\{J_i^{(k)}\}_{i\in\mathbb{N}} \subset \mathcal{K}_k$ with $\|J_i^{(k)}\| \leq 1$ for all $i\in\mathbb{N}$. Using the operators $J_i^{(k)}$, we define the following metric $\eta_k(\cdot, \cdot)$ on the unit ball of \mathcal{L}_k^1 . For $\gamma^{(k)}, \tilde{\gamma}^{(k)} \in \mathcal{L}_k^1$ with $\|\gamma^{(k)}\|_{\mathcal{L}^1}, \|\tilde{\gamma}^{(k)}\|_{\mathcal{L}^1} \leq 1$, we set

$$\eta_k(\gamma^{(k)}, \tilde{\gamma}^{(k)}) := \sum_{i=1}^{\infty} \frac{1}{2^i} \left| \text{tr} J_i^{(k)} (\gamma^{(k)} - \tilde{\gamma}^{(k)}) \right|. \quad (5.5)$$

Hence, a uniformly bounded sequence $\{\gamma_N^{(k)}\}_{N\in\mathbb{N}} \subset \mathcal{L}_k^1$ with $\|\gamma_N^{(k)}\|_{\mathcal{L}^1} \leq 1$ for all $N\in\mathbb{N}$, converges to some $\gamma^{(k)}$ as $N \rightarrow \infty$ with respect to the weak* topology of \mathcal{L}_k^1 if and only if

$\eta_k(\gamma_N^{(k)}, \gamma^{(k)}) \rightarrow 0$ as $N \rightarrow \infty$ (see Théorème III.25 in [5]).

For arbitrary $T > 0$ let $C([0, T]; \mathcal{L}_k^1)$ be the space of functions of $t \in [0, T]$ with values in \mathcal{L}_k^1 which are continuous with respect to the metric η_k . On $C([0, T]; \mathcal{L}_k^1)$ we define the metric

$$\widehat{\eta}_k(\gamma^{(k)}(\cdot), \widetilde{\gamma}^{(k)}(\cdot)) := \sup_{t \in [0, T]} \eta_k(\gamma^{(k)}(t), \widetilde{\gamma}^{(k)}(t)). \quad (5.6)$$

Last, we denote by τ_{prod} the topology on the space $\bigoplus_{k \in \mathbb{N}} C([0, T]; \mathcal{L}_k^1)$ given by the product of the topologies generated by the metrics $\widehat{\eta}_k$ on $C([0, T]; \mathcal{L}_k^1)$.

Remark 5.2. Convergence of the sequence $(\Gamma_{N,t})_{N \in \mathbb{N}}$ to $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \in \mathbb{N}}$ with respect to the topology τ_{prod} is equivalent to the statement that, for every fixed $k \in \mathbb{N}$ and for every fixed compact operator $J^{(k)} \in \mathcal{K}_k$,

$$\text{tr } J^{(k)} \left(\gamma_{N,t}^{(k)} - \gamma_{\infty,t}^{(k)} \right) \rightarrow 0 \quad (5.7)$$

as $N \rightarrow \infty$, uniformly in t for $t \in [0, T]$.

Precompactness of the sequence $(\Gamma_{N,t})_{N \in \mathbb{N}}$ with respect to the topology τ_{prod} means therefore that for every strictly increasing sequence $\{M_j\}_{j \in \mathbb{N}} \subset \mathbb{N}$ there exists a subsequence $\{N_j\}_{j \in \mathbb{N}} \subset \{M_j\}_{j \in \mathbb{N}}$ and a limit point $\Gamma_{\infty,t}$ such that $\Gamma_{N_j,t} \rightarrow \Gamma_{\infty,t}$ as $j \rightarrow \infty$ in the sense (5.7).

Owing to the metric structure introduced on the space $\bigoplus_{k \in \mathbb{N}} C([0, T]; \mathcal{L}_k^1)$, we are now in a position to invoke the Arzela-Ascoli Theorem to prove the precompactness of the sequence $\{\Gamma_{N,t}\}_{N \in \mathbb{N}}$ with respect to the topology τ_{prod} .

Proposition 5.3. *Fix an arbitrary $T > 0$. Suppose that $V \in L^\infty(\mathbb{R}^3)$ and that the magnetic vector potential $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ satisfies assumption **(A)**. Then the sequence $(\Gamma_{N,t})_{N \in \mathbb{N}} \subset \bigoplus_{k \in \mathbb{N}} C([0, T]; \mathcal{L}_k^1)$ with $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ is precompact with respect to the topology τ_{prod} .*

Proof. By a standard “choice of the diagonal subsequence” argument, it is enough to prove the precompactness of $\{\gamma_{N,t}^{(k)}\}_{N \geq k}$ for every fixed $k \in \mathbb{N}$ with respect to the metric $\widehat{\eta}_k$ on $C([0, T]; \mathcal{L}_k^1)$. To this end we would like to invoke the Arzela-Ascoli Theorem. The elements of the sequence $\{\gamma_{N,t}^{(k)}\}_{N \geq k}$ are uniformly bounded in trace norm by 1. It therefore remains to prove the equicontinuity of the sequence with respect to the metric $\widehat{\eta}_k$, for which the next lemma gives a criterion.

Lemma 5.4. *Fix $k \in \mathbb{N}$ and $T > 0$. A sequence $\{\gamma_{N,t}^{(k)}\}_{N \geq k} \subset \mathcal{L}_k^1$ with $\gamma_{N,t}^{(k)} \geq 0$ and $\text{tr } \gamma_{N,t}^{(k)} = 1$ for all $t \in [0, T]$ and $N \geq k$, is equicontinuous in $C([0, T]; \mathcal{L}_k^1)$ with respect to the metric $\widehat{\eta}_k$, if and only if there exists a dense subset \mathcal{J}_k of \mathcal{K}_k such that for any $J^{(k)} \in \mathcal{J}_k$ and for every $\varepsilon > 0$ there exists a $\delta > 0$ such that*

$$\sup_{N \geq 1} \left| \text{tr } J^{(k)} \left(\gamma_{N,t}^{(k)} - \gamma_{N,s}^{(k)} \right) \right| \leq \varepsilon \quad (5.8)$$

for all $t, s \in [0, T]$ with $|t - s| \leq \delta$.

Proof of Lemma 5.4. The statement is Lemma 6.2 in [14], its proof is analogous to the one of Lemma 9.2 in [9]. \square

Identifying operators with their kernels, we choose the set $\mathcal{J}^{(k)} = H_A^1(\mathbb{R}^{3k}) \times H_A^1(\mathbb{R}^{3k})$ for the proof of equicontinuity. $\mathcal{J}^{(k)}$ is dense in the set of compact operators \mathcal{K}_k , because it contains all operators with kernels in $C_c^\infty(\mathbb{R}^{3k}) \times C_c^\infty(\mathbb{R}^{3k})$. These are dense in $L^2(\mathbb{R}^{3k}) \times L^2(\mathbb{R}^{3k})$, i.e. the set of Hilbert-Schmidt operators $\mathcal{L}_k^2 \equiv \mathcal{L}^2(L^2(\mathbb{R}^{3k}))$, which are in turn dense in \mathcal{K}_k .

For any $s \leq t$, we rewrite the BBGKY hierarchy in integral form

$$\begin{aligned} \gamma_{N,t}^{(k)} &= \gamma_{N,s}^{(k)} - i \sum_{j=1}^k \int_s^t dr [h_j, \gamma_{N,r}^{(k)}] - i \frac{1}{N} \sum_{i<j}^k \int_s^t dr [V(x_i - x_j), \gamma_{N,r}^{(k)}] \\ &\quad - i \left(1 - \frac{k}{N}\right) \sum_{j=1}^k \int_s^t dr \operatorname{tr}_{[k+1]} [V(x_j - x_{k+1}), \gamma_{N,r}^{(k+1)}]. \end{aligned} \quad (5.9)$$

Multiplying the last equation with a $J^{(k)} \in \mathcal{J}^{(k)}$ and taking the trace, we obtain the bound

$$\begin{aligned} & \left| \operatorname{tr} J^{(k)} (\gamma_{N,t}^{(k)} - \gamma_{N,s}^{(k)}) \right| \\ & \leq \sum_{j=1}^k \int_s^t dr \left| \operatorname{tr} J^{(k)} [h_j, \gamma_{N,r}^{(k)}] \right| \\ & \quad + \frac{1}{N} \sum_{i<j}^k \int_s^t dr \left| \operatorname{tr} J^{(k)} [V(x_i - x_j), \gamma_{N,r}^{(k)}] \right| \\ & \quad + \left(1 - \frac{k}{N}\right) \sum_{j=1}^k \int_s^t dr \left| \operatorname{tr} J^{(k)} \operatorname{tr}_{[k+1]} [V(x_j - x_{k+1}), \gamma_{N,r}^{(k+1)}] \right| \\ & \leq \left(\sum_{j=1}^k \sup_{r \in [s,t]} \left\{ \operatorname{tr} \left| J^{(k)} [h_j, \gamma_{N,r}^{(k)}] \right| \right\} + (k^2 + 2k) \|J^{(k)}\| \|V\| \right) |t - s|. \end{aligned} \quad (5.10)$$

We will next show that the expression $\operatorname{tr} \left| J^{(k)} [h_j, \gamma_{N,t}^{(k)}] \right|$ is uniformly bounded in $N \in \mathbb{N}, t \in [0, T]$ and $j \in \{1, \dots, N\}$. This gives the equicontinuity of the sequence $\{\gamma_{N,t}^{(k)}\}_{N \geq k}$ by Lemma 5.4.

Let $N \in \mathbb{N}, t \in [0, T]$ and $j \in \{1, \dots, N\}$ be arbitrary and denote $S_j = \sqrt{1 + h_j}$. Then

$$\begin{aligned} \left| \operatorname{tr} J^{(k)} [h_j, \gamma_{N,t}^{(k)}] \right| &\leq \left| \operatorname{tr} J^{(k)} h_j \gamma_{N,t}^{(k)} \right| + \left| \operatorname{tr} J^{(k)} \gamma_{N,t}^{(k)} h_j \right| \\ &\leq \left\| S_j^{-1} J^{(k)} S_j \right\| \left\| S_j^{-1} h_j S_j^{-1} \right\| \left| \operatorname{tr} S_j \gamma_{N,t}^{(k)} S_j \right| \\ &\quad + \left\| S_j J^{(k)} S_j^{-1} \right\| \left\| S_j^{-1} h_j S_j^{-1} \right\| \left| \operatorname{tr} S_j \gamma_{N,t}^{(k)} S_j \right|. \end{aligned} \quad (5.11)$$

Now we show that each of the factors of the two summands in the last line of (5.11) is

uniformly bounded. For $J^{(k)} \in \mathcal{J}^{(k)}$ we have

$$\begin{aligned}
\|J^{(k)}S_j\|_{\mathcal{L}^2}^2 &= \text{tr}(J^{(k)}S_j)^*J^{(k)}S_j \\
&= \text{tr}J^{(k)*}J^{(k)}S_j^2 \\
&= \int d\mathbf{x}_k d\mathbf{x}'_k |J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k)|^2 + \int d\mathbf{x}_k d\mathbf{x}'_k |(-i\nabla'_j + A(x'_j))J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k)|^2 \\
&< \infty
\end{aligned} \tag{5.12}$$

by the choice of $\mathcal{J}^{(k)}$. Thus $J^{(k)}S_j$ is a Hilbert-Schmidt operator, i.e. in particular bounded, and therefore $S_j^{-1}J^{(k)}S_j$ is bounded. Analogously, it follows that $S_jJ^{(k)}S_j^{-1}$ is bounded.

Moreover $\|S_j^{-1}h_jS_j^{-1}\| < 1$ by functional calculus and

$$\text{tr}\left|S_j\gamma_{N,t}^{(k)}S_j\right| = \|\psi_{N,t}\|_2^2 + \|(-i\nabla_j + A)\psi_{N,t}\|_2^2 = 1 + \|(-i\nabla_j + A)\psi_{N,t}\|_2^2. \tag{5.13}$$

To obtain a uniform bound on $\|(-i\nabla_j + A)\psi_{N,t}\|_2^2$ we use the conservation of mass and energy for the many-body linear Schrödinger equation (1.4). The initial state $\psi_N = \varphi^{\otimes N}$ with $\varphi \in H_A^1(\mathbb{R}^3)$, $\|\varphi\|_2 = 1$, has energy

$$\begin{aligned}
E_N &= \langle \psi_N, H_N \psi_N \rangle \\
&= \sum_{j=1}^N \|(-i\nabla_j + A)\psi_N\|_2^2 + \frac{1}{N} \sum_{i<j}^N \int d\mathbf{x}_N V(x_i - x_j) |\psi_N(\mathbf{x}_N)|^2 \\
&= N\|(-i\nabla + A)\varphi\|_2^2 + \frac{N-1}{2} \int dx_1 dx_2 V(x_1 - x_2) |\varphi(x_1)|^2 |\varphi(x_2)|^2 \\
&\leq NC',
\end{aligned} \tag{5.14}$$

where we used the permutation symmetry of ψ_N . The conservation of mass and energy for the Schrödinger equation then implies for all $t \in [0, T]$ that

$$\begin{aligned}
E_N &= \langle \psi_{N,t}, H_N \psi_{N,t} \rangle \\
&= \sum_{j=1}^N \|(-i\nabla_j + A(x_j))\psi_{N,t}\|_2^2 + \frac{1}{N} \sum_{i<j}^N \int d\mathbf{x}_N V(x_i - x_j) |\psi_{N,t}(\mathbf{x}_N)|^2 \\
&\geq \sum_{j=1}^N \|(-i\nabla_j + A(x_j))\psi_{N,t}\|_2^2 - \frac{1}{N} \|V\|_\infty \sum_{i<j}^N \|\psi_{N,t}\|_2^2 \\
&= \sum_{j=1}^N \|(-i\nabla_j + A(x_j))\psi_{N,t}\|_2^2 - \frac{N-1}{2} \|V\|_\infty.
\end{aligned} \tag{5.15}$$

Thus for arbitrary $j \in \{1, \dots, N\}$ we have by permutation symmetry,

$$\begin{aligned}
\|(-i\nabla_j + A(x_j))\psi_{N,t}\|_2^2 &= \frac{1}{N} \sum_{l=1}^N \|(-i\nabla_l + A(x_l))\psi_{N,t}\|_2^2 \\
&\leq \frac{1}{N} (E_N + \frac{N-1}{2} \|V\|_\infty) \\
&\leq \frac{1}{N} (NC' + \frac{N-1}{2} \|V\|_\infty) \\
&\leq C
\end{aligned} \tag{5.16}$$

for all N and at all times $t \in [0, T]$. This completes the proof of the precompactness of the sequence $\{\gamma_{N,t}^{(k)}\}_{N \geq k}$ with respect to the metric $\widehat{\eta}_k$ on $C([0, T]; \mathcal{L}_k^1)$. \square

Moreover, we prove the following properties of limit points of the sequence $(\Gamma_{N,t})_{N \in \mathbb{N}}$, which we will need later on.

Proposition 5.5. *Let $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \in \mathbb{N}}$ be an arbitrary limit point of the sequence $(\Gamma_{N,t})_{N \in \mathbb{N}} \subset \bigoplus_{k \in \mathbb{N}} C([0, T]; \mathcal{L}_k^1)$ with respect to the topology τ_{prod} . Then $\gamma_{\infty,t}^{(k)}$ is symmetric with respect to permutations, non-negative and such that*

$$\mathrm{tr} \gamma_{\infty,t}^{(k)} \leq 1 \quad (5.17)$$

for every $k \geq 1$.

Proof. Suppose that $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \in \mathbb{N}} \in \bigoplus_{k \in \mathbb{N}} C([0, T]; \mathcal{L}_k^1)$ is a limit point of $\Gamma_{N,t}$ with respect to τ_{prod} . Then for any $k \in \mathbb{N}$, $\gamma_{\infty,t}^{(k)} \in C([0, T]; \mathcal{L}_k^1)$ is a limit point of $\{\gamma_{N,t}^{(k)}\}_{N \geq k}$ in the sense (5.7). The bound

$$\mathrm{tr} \left| \gamma_{\infty,t}^{(k)} \right| \leq 1 \quad (5.18)$$

follows because the norm can only drop in the weak limit.

To prove that $\gamma_{\infty,t}^{(k)}$ is non-negative we observe that, for an arbitrary $\varphi \in L^2(\mathbb{R}^{3k})$ with $\|\varphi\|_2 = 1$, the orthogonal projection $|\varphi\rangle\langle\varphi|$ is in \mathcal{K}_k and hence

$$\langle\varphi, \gamma_{\infty,t}^{(k)} \varphi\rangle = \mathrm{tr} |\varphi\rangle\langle\varphi| \gamma_{\infty,t}^{(k)} = \lim_{j \rightarrow \infty} \mathrm{tr} |\varphi\rangle\langle\varphi| \gamma_{N_j,t}^{(k)} = \lim_{j \rightarrow \infty} \langle\varphi, \gamma_{N_j,t}^{(k)} \varphi\rangle \geq 0 \quad (5.19)$$

for an appropriate subsequence $(N_j)_{j \in \mathbb{N}}$ with $N_j \rightarrow \infty$ as $j \rightarrow \infty$.

Last, we show that $\gamma_{\infty,t}^{(k)}$ is symmetric with respect to permutations. For a permutation π of $\{1, \dots, k\}$, we denote by Ξ_π the operator on $L^2(\mathbb{R}^{3k})$ defined by

$$(\Xi_\pi \varphi) = \varphi(x_{\pi(1)}, \dots, x_{\pi(k)}). \quad (5.20)$$

Then the permutation symmetry of $\gamma_{\infty,t}^{(k)}$ is defined by asserting that

$$\Xi_\pi \gamma_{\infty,t}^{(k)} \Xi_\pi^{-1} = \gamma_{\infty,t}^{(k)} \quad (5.21)$$

holds for every permutation π . To prove (5.21) we note that, for an arbitrary $J^{(k)} \in \mathcal{K}_k$ and a permutation π of $\{1, \dots, k\}$, we have, for an appropriate subsequence $N_j \rightarrow \infty$ as $j \rightarrow \infty$,

$$\begin{aligned} \mathrm{tr} J^{(k)} \gamma_{\infty,t}^{(k)} &= \lim_{j \rightarrow \infty} \mathrm{tr} J^{(k)} \gamma_{N_j,t}^{(k)} = \lim_{j \rightarrow \infty} \mathrm{tr} J^{(k)} \Xi_\pi \gamma_{N_j,t}^{(k)} \Xi_\pi^{-1} = \lim_{j \rightarrow \infty} \Xi_\pi^{-1} J^{(k)} \Xi_\pi \gamma_{N_j,t}^{(k)} \\ &= \mathrm{tr} \Xi_\pi^{-1} J^{(k)} \Xi_\pi \gamma_{\infty,t}^{(k)} = \mathrm{tr} J^{(k)} \Xi_\pi \gamma_{\infty,t}^{(k)} \Xi_\pi^{-1}, \end{aligned} \quad (5.22)$$

where we used that $\Xi_\pi^{-1} J^{(k)} \Xi_\pi \in \mathcal{K}_k$ for every $J^{(k)} \in \mathcal{K}_k$ and every permutation π . \square

Step 2: Convergence

In this second step we characterise the weak limit points of the sequence $(\Gamma_{N,t})_{N \in \mathbb{N}}$ as solutions to the infinite hierarchy of equations (5.3).

Proposition 5.6. *Suppose that $V \in L^\infty(\mathbb{R}^3)$ such that $V(x) \rightarrow 0$ as $|x| \rightarrow \infty$ and that the magnetic vector potential $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ satisfies assumption **(A)**. Assume moreover that $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \in \mathbb{N}} \in \bigoplus_{k \in \mathbb{N}} C([0, T]; \mathcal{L}_k^1)$ is a limit point of the sequence $(\Gamma_{N,t})_{N \in \mathbb{N}}$ with respect to the topology τ_{prod} . Then $\gamma_{\infty,0}^{(k)} = |\varphi\rangle\langle\varphi|^{\otimes k}$ and*

$$\gamma_{\infty,t}^{(k)} = \mathcal{U}^{(k)}(t)\gamma_{\infty,0}^{(k)} + \int_0^t ds \mathcal{U}^{(k)}(t-s)B^{(k)}\gamma_{\infty,s}^{(k+1)} \quad (5.23)$$

for all $k \in \mathbb{N}$. Here $\mathcal{U}^{(k)}(t)$ and $B^{(k)}$ are defined as in (4.7) and, respectively, in (4.9).

Proof. Passing to a subsequence we can assume that $\Gamma_{N,t} \rightarrow \Gamma_{\infty,t}$ as $N \rightarrow \infty$, with respect to the topology τ_{prod} . This implies immediately that $\gamma_{\infty,0}^{(k)} = |\varphi\rangle\langle\varphi|^{\otimes k}$. To show (5.23), it is enough to prove that for every fixed $k \in \mathbb{N}$ and for every fixed $J^{(k)}$ from a dense subset $\mathcal{J}^{(k)}$ of \mathcal{K}_k ,

$$\text{tr } J^{(k)}\gamma_{\infty,t}^{(k)} = \text{tr } J^{(k)}\mathcal{U}^{(k)}(t)\gamma_{\infty,0}^{(k)} + \int_0^t ds \text{tr } J^{(k)}\mathcal{U}^{(k)}(t-s)B^{(k)}\gamma_{\infty,s}^{(k+1)}. \quad (5.24)$$

For what follows, we choose $\mathcal{J}^{(k)} = \mathcal{L}_k^2$ as the set of Hilbert-Schmidt operators on $L^2(\mathbb{R}^{3k})$, which are dense in \mathcal{K}_k . We start from the integral form (4.6) of the BBGKY hierarchy of equations for the marginals $\{\gamma_{N,t}^{(k)}\}_{k=1}^N$. For $k \in \{1, \dots, N\}$, we multiply the corresponding equation from the hierarchy with a fixed, but arbitrary $J^{(k)} \in \mathcal{J}^{(k)}$ and take the trace. This leads to the relations

$$\begin{aligned} \text{tr } J^{(k)}\gamma_{N,t}^{(k)} &= \text{tr } J^{(k)}\mathcal{U}^{(k)}(t)\gamma_N^{(k)} - i \frac{1}{N} \sum_{i < j}^k \int_0^t ds \text{tr } J^{(k)}\mathcal{U}^{(k)}(t-s)[V(x_i - x_j), \gamma_{N,s}^{(k)}] \\ &\quad + \frac{N-k}{N} \int_0^t ds \text{tr } J^{(k)}\mathcal{U}^{(k)}(t-s)B^{(k)}\gamma_{N,s}^{(k+1)}. \end{aligned} \quad (5.25)$$

By assumption the left-hand side of (5.25) converges to the one of (5.24) as $N \rightarrow \infty$. Also, the first term on the right-hand side of (5.25) coincides with the one of (5.24). So the claim follows if we can show that

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i < j}^k \int_0^t ds \text{tr } J^{(k)}\mathcal{U}^{(k)}(t-s)[V(x_i - x_j), \gamma_{N,s}^{(k)}] = 0 \quad (5.26)$$

and that

$$\lim_{N \rightarrow \infty} \left(1 - \frac{k}{N}\right) \int_0^t ds \text{tr } J^{(k)}\mathcal{U}^{(k)}(t-s)B^{(k)}\gamma_{N,s}^{(k+1)} = \int_0^t ds \text{tr } J^{(k)}\mathcal{U}^{(k)}(t-s)B^{(k)}\gamma_{\infty,s}^{(k+1)}. \quad (5.27)$$

The limit (5.26) follows immediately from the estimate

$$\left| \frac{1}{N} \sum_{i < j}^k \int_0^t ds \text{tr } J^{(k)}\mathcal{U}^{(k)}(t-s)[V(x_i - x_j), \gamma_{N,s}^{(k)}] \right| \leq \frac{k^2}{N} \|J^{(k)}\| \|V\| |t|. \quad (5.28)$$

Moreover, observe that

$$\left| \frac{k}{N} \int_0^t ds \text{tr } J^{(k)}\mathcal{U}^{(k)}(t-s)B^{(k)}\gamma_{N,s}^{(k+1)} \right| \leq \frac{2k^2}{N} \|J^{(k)}\| \|V\| |t| \rightarrow 0 \quad (5.29)$$

as $N \rightarrow \infty$. It therefore remains to show

$$\lim_{N \rightarrow \infty} \int_0^t ds \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) B^{(k)} (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}) = 0. \quad (5.30)$$

We have

$$\begin{aligned} & \int_0^t ds \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) B^{(k)} (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}) \\ &= -i \sum_{j=1}^k \int_0^t ds \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) \operatorname{tr}_{[k+1]} [V(x_j - x_{k+1}), (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)})] \\ &= -i \sum_{j=1}^k \int_0^t ds \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) [V(x_j - x_{k+1}), (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)})] \\ &= -ik \int_0^t ds \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) V(x_1 - x_{k+1}) (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}) \\ & \quad + ik \int_0^t ds \operatorname{tr} V(x_1 - x_{k+1}) J^{(k)} \mathcal{U}^{(k)}(t-s) (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}), \end{aligned} \quad (5.31)$$

where in the last step, we used the cyclicity of the trace and the permutation symmetry of $\gamma_{N,s}^{(k+1)}$ and $\gamma_{\infty,s}^{(k+1)}$. In order to show that the two terms in the last line of (5.31) vanish in the limit $N \rightarrow \infty$, we would like to use the weak* - convergence in \mathcal{L}_{k+1}^1 of $\gamma_{N,s}^{(k+1)} \rightharpoonup \gamma_{\infty,s}^{(k+1)}$ as $N \rightarrow \infty$. We know that the operator $J^{(k)}$ is compact on $L^2(\mathbb{R}^{3k})$. However, the operators $J^{(k)} \mathcal{U}^{(k)}(t-s) V(x_1 - x_{k+1})$ and $V(x_1 - x_{k+1}) J^{(k)} \mathcal{U}^{(k)}(t-s)$ are *not* necessarily compact operators on $L^2(\mathbb{R}^{3(k+1)})$, so that a straightforward application of the weak* - convergence in the sense (5.7) is not possible. To overcome this obstacle, we have to introduce several cut-offs and exploit energy conservation.

We now show that the first term in the last line of (5.31) vanishes in the limit $N \rightarrow \infty$. The second term in the last line of (5.31) can be treated in a similar way. This then completes the proof of Proposition 5.6.

To this end we notice that the vanishing of

$$\int_0^t ds \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) V(x_1 - x_{k+1}) (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}) \quad (5.32)$$

in the limit $N \rightarrow \infty$ follows by dominated convergence, if we can show that for all $s \in [0, t]$

$$\operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) V(x_1 - x_{k+1}) (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}) \quad (5.33)$$

vanishes as $N \rightarrow \infty$. We found two different proofs to show this. We now present one of the proofs, the other one is outlined in Remark 5.7 below. Recall the notation $S_{k+1} = \sqrt{1 + h_{k+1}}$. For $n > 0$ we introduce

$$V_{<n}(x) = V(x) \mathbb{1}_{\{|x| < n\}} \quad \text{and} \quad V_{\geq n}(x) = V(x) \mathbb{1}_{\{|x| \geq n\}}. \quad (5.34)$$

Let $\varepsilon > 0$ be arbitrary. Choose $n > 0$ large enough such that $\|V_{\geq n}\|_{\infty} \leq \varepsilon$. This is possible owing to the assumption that $V(x) \rightarrow 0$ as $|x| \rightarrow \infty$. Applying a cut-off in momentum space,

then a cut-off to the potential V and then another cut-off in momentum space, we can write (5.33) as

$$\begin{aligned} & \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) V(x_1 - x_{k+1}) (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}) \\ = & \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) V(x_1 - x_{k+1}) \left(1 - \frac{1}{1 + \varepsilon S_{k+1}} \right) (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}) \end{aligned} \quad (I)$$

$$+ \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) V_{\geq n}(x_1 - x_{k+1}) \frac{1}{1 + \varepsilon S_{k+1}} (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}) \quad (II)$$

$$+ \operatorname{tr} \left(1 - \frac{1}{1 + \varepsilon S_{k+1}} \right) J^{(k)} \mathcal{U}^{(k)}(t-s) V_{< n}(x_1 - x_{k+1}) \frac{1}{1 + \varepsilon S_{k+1}} (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}) \quad (III)$$

$$+ \operatorname{tr} \frac{1}{1 + \varepsilon S_{k+1}} J^{(k)} \mathcal{U}^{(k)}(t-s) V_{< n}(x_1 - x_{k+1}) \frac{1}{1 + \varepsilon S_{k+1}} (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}). \quad (IV)$$

(5.35)

We can estimate the term (I) in (5.35) using energy conservation:

$$\begin{aligned} |(I)| & \leq \varepsilon \|J^{(k)} \mathcal{U}^{(k)}(t-s)\| \|V\| \left\| \frac{1}{1 + \varepsilon S_{k+1}} \right\| \left(\operatorname{tr} \left| S_{k+1} \gamma_{N,s}^{(k+1)} \right| + \operatorname{tr} \left| S_{k+1} \gamma_{\infty,s}^{(k+1)} \right| \right) \\ & \leq \varepsilon \|J^{(k)}\| \|V\| \left(\operatorname{tr} \left| S_{k+1} \gamma_{N,s}^{(k+1)} S_{k+1} \right| + \operatorname{tr} \left| S_{k+1} \gamma_{\infty,s}^{(k+1)} S_{k+1} \right| \right) \\ & \leq \varepsilon \|J^{(k)}\| \|V\| C, \end{aligned} \quad (5.36)$$

where $C > 0$ is independent of N and $s \in [0, t]$. Here we used the monotonicity of the operator square root (see the remark to Proposition 2.2.13 in [4]) in the second line. We exploited energy conservation in the third line to obtain a bound on $\operatorname{tr} \left| S_{k+1} \gamma_{N,s}^{(k+1)} S_{k+1} \right|$ uniform in N and time $s \in [0, t]$ and thus also on $\operatorname{tr} \left| S_{k+1} \gamma_{\infty,s}^{(k+1)} S_{k+1} \right|$ (see (5.13) – (5.16) for more details).

Now the second term (II) in (5.35) can be bounded by

$$|(II)| \leq \|J^{(k)}\| \|V_{\geq n}\|_{\infty} \left\| \frac{1}{1 + \varepsilon S_{k+1}} \right\| \operatorname{tr} \left| \gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)} \right| \leq \varepsilon 2 \|J^{(k)}\|. \quad (5.37)$$

The third term (III) in (5.35) can again be bounded using energy conservation:

$$\begin{aligned} |(III)| & \leq \varepsilon \|J^{(k)}\| \|V_{< n}\| \left\| \frac{1}{1 + \varepsilon S_{k+1}} \right\| \left(\operatorname{tr} \left| \gamma_{N,s}^{(k+1)} S_{k+1} \right| + \operatorname{tr} \left| \gamma_{\infty,s}^{(k+1)} S_{k+1} \right| \right) \left\| \frac{1}{1 + \varepsilon S_{k+1}} \right\| \\ & \leq \varepsilon \|J^{(k)}\| \|V\| \left(\operatorname{tr} \left| S_{k+1} \gamma_{N,s}^{(k+1)} S_{k+1} \right| + \operatorname{tr} \left| S_{k+1} \gamma_{\infty,s}^{(k+1)} S_{k+1} \right| \right) \\ & \leq \varepsilon \|J^{(k)}\| \|V\| C. \end{aligned} \quad (5.38)$$

In order to control the fourth term (IV) in (5.35), we use the weak* - convergence $\gamma_{N,s}^{(k+1)} \rightharpoonup \gamma_{\infty,s}^{(k+1)}$ as $N \rightarrow \infty$ in \mathcal{L}_{k+1}^1 . We show below that

$$\frac{1}{1 + \varepsilon S_{k+1}} J^{(k)} \mathcal{U}^{(k)}(t-s) V_{< n}(x_1 - x_{k+1}) \frac{1}{1 + \varepsilon S_{k+1}} \quad (5.39)$$

is a compact $(k+1)$ -particle operator. Thus, we can choose N large enough so that $|(IV)| \leq \varepsilon$. Collecting the estimates of the terms (I) - (IV), we obtain that for arbitrary $\varepsilon > 0$, we can choose N large enough so that

$$\left| \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) V(x_1 - x_{k+1}) (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}) \right| \leq (2 \|J^{(k)}\| \|V\| C + 2 \|J^{(k)}\| + 1) \varepsilon. \quad (5.40)$$

Since $\varepsilon > 0$ was chosen arbitrarily, this implies for all $s \in [0, t]$ the vanishing of the term (5.33) as $N \rightarrow \infty$, which completes the proof.

It remains to show the crucial ingredient of the above proof, namely the compactness of the $(k+1)$ -particle operator (5.39). We denote $J_s^{(k)} \equiv J^{(k)} \mathcal{U}^{(k)}(t-s)$. Then $J_s^{(k)} \in \mathcal{L}_k^2$ is a Hilbert-Schmidt operator, because $J^{(k)} \in \mathcal{L}_k^2$ and $\mathcal{U}^{(k)}(t-s)$ is bounded. We have

$$\begin{aligned} & \frac{1}{1 + \varepsilon S_{k+1}} J_s^{(k)} V_{<n}(x_1 - x_{k+1}) \frac{1}{1 + \varepsilon S_{k+1}} \\ &= \left(\frac{1}{1 + \varepsilon S_{k+1}} \varepsilon S_{k+1} \right) \frac{1}{\varepsilon} \left(\frac{1}{S_{k+1}} J_s^{(k)} V_{<n}(x_1 - x_{k+1}) \frac{1}{S_{k+1}} \right) \frac{1}{\varepsilon} \left(\varepsilon S_{k+1} \frac{1}{1 + \varepsilon S_{k+1}} \right). \end{aligned} \quad (5.41)$$

By functional calculus, the operators in the first and third parentheses on the right-hand side of (5.41) are bounded. To show that the operator on the left-hand side of (5.41) is compact, it is therefore sufficient to show that the operator in the second parentheses on the right-hand side of (5.41) is compact. We denote it by T and prove that it is actually a Hilbert-Schmidt operator and hence, in particular compact. To this end we compute the Hilbert-Schmidt norm of T :

$$\begin{aligned} & \operatorname{tr} T^* T \\ &= \operatorname{tr} \frac{1}{S_{k+1}} V_{<n}(x_1 - x_{k+1}) (J_s^{(k)})^* \frac{1}{S_{k+1}^2} J_s^{(k)} V_{<n}(x_1 - x_{k+1}) \frac{1}{S_{k+1}} \\ &= \operatorname{tr} V_{<n}(x_1 - x_{k+1}) (J_s^{(k)})^* \frac{1}{S_{k+1}^2} J_s^{(k)} V_{<n}(x_1 - x_{k+1}) \frac{1}{S_{k+1}^2} \\ &= \operatorname{tr} V_{<n}(x_1 - x_{k+1}) (J_s^{(k)})^* \frac{1}{1 + h_{k+1}} J_s^{(k)} V_{<n}(x_1 - x_{k+1}) \frac{1}{1 + h_{k+1}} \\ &= \int d\mathbf{x}_k dx_{k+1} d\mathbf{y}_k dy_{k+1} V_{<n}(x_1 - x_{k+1}) \overline{J_s^{(k)}(\mathbf{y}_k; \mathbf{x}_k)} \left(\frac{1}{1 + h_{k+1}} \right) (x_{k+1}; y_{k+1}) \times \\ & \quad \times J_s^{(k)}(\mathbf{y}_k; \mathbf{x}_k) V_{<n}(x_1 - x_{k+1}) \left(\frac{1}{1 + h_{k+1}} \right) (y_{k+1}; x_{k+1}) \\ &= \int d\mathbf{x}_k dx_{k+1} d\mathbf{y}_k dy_{k+1} \left| J_s^{(k)}(\mathbf{y}_k; \mathbf{x}_k) \right|^2 \left| V_{<n}(x_1 - x_{k+1}) \right|^2 \left| \left(\frac{1}{1 + h_{k+1}} \right) (x_{k+1}; y_{k+1}) \right|^2 \\ &\leq \int d\mathbf{x}_k dx_{k+1} d\mathbf{y}_k dy_{k+1} \left| J_s^{(k)}(\mathbf{y}_k; \mathbf{x}_k) \right|^2 \left| V_{<n}(x_1 - x_{k+1}) \right|^2 \left| \left(\frac{1}{1 - \Delta_{k+1}} \right) (x_{k+1} - y_{k+1}) \right|^2 \\ &= \int d\mathbf{x}_k d\mathbf{y}_k \left| J_s^{(k)}(\mathbf{y}_k; \mathbf{x}_k) \right|^2 \int dx_{k+1} \left| V_{<n}(x_1 - x_{k+1}) \right|^2 \int dy_{k+1} \left| \left(\frac{1}{1 - \Delta_{k+1}} \right) (x_{k+1} - y_{k+1}) \right|^2. \end{aligned} \quad (5.42)$$

Here we used the non-relativistic diamagnetic inequality (8.12) in the penultimate line. The last line of (5.42) is finite due to the following reasoning: The translationally invariant kernel $\left(\frac{1}{1 - \Delta} \right) (x - y) = \frac{1}{4\pi} \frac{e^{-|x-y|}}{|x-y|}$ is square-integrable in y_{k+1} . Moreover, $\int dx_{k+1} |V_{<n}(x_1 - x_{k+1})|^2$

is finite because $V_{<n}$ is bounded and has finite support. Since $J_s^{(k)} \in \mathcal{L}_k^2$ is a k -particle Hilbert-Schmidt operator, $\int d\mathbf{x}_k d\mathbf{y}_k |J_s^{(k)}(\mathbf{y}_k; \mathbf{x}_k)|^2$ is also finite. Thus, T is a k -particle Hilbert-Schmidt operator, which completes the proof. \square

Remark 5.7. The crucial step in the proof of Proposition 5.6 is to show that the term (5.33) vanishes as $N \rightarrow \infty$. To this end we introduced several cut-offs and then showed the compactness of the $(k+1)$ -particle operator (5.39) in order to make use of the weak* - convergence $\gamma_{N,s}^{(k+1)} \rightharpoonup \gamma_{\infty,s}^{(k+1)}$ as $N \rightarrow \infty$ in \mathcal{L}_{k+1}^1 .

In a different approach to show the vanishing of the term (5.33), we introduce a cut-off in momentum space to write (5.33) as follows:

$$\begin{aligned} & \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) V(x_1 - x_{k+1}) (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}) \\ = & \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) V(x_1 - x_{k+1}) \left(1 - \frac{1}{1 + \varepsilon S_{k+1}} \right) (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}) \end{aligned} \quad (I)$$

$$+ \operatorname{tr} J^{(k)} \mathcal{U}^{(k)}(t-s) V(x_1 - x_{k+1}) \frac{1}{1 + \varepsilon S_{k+1}} (\gamma_{N,s}^{(k+1)} - \gamma_{\infty,s}^{(k+1)}). \quad (II)$$

(5.43)

The first term (I) in (5.43) can be controlled by energy conservation. In order to show that the second term (II) in (5.43) vanishes as $N \rightarrow \infty$, we make use of the weak* - convergence $\gamma_{N,s}^{(k+1)} \rightharpoonup \gamma_{\infty,s}^{(k+1)}$ as $N \rightarrow \infty$ in \mathcal{L}_{k+1}^1 . To this end we have to prove that the operator

$$J^{(k)} \mathcal{U}^{(k)}(t-s) V(x_1 - x_{k+1}) \frac{1}{1 + \varepsilon S_{k+1}} \quad (5.44)$$

is a compact $(k+1)$ -particle operator on $L^2(\mathbb{R}^{3(k+1)})$. We know that $J^{(k)} \mathcal{U}^{(k)}(t-s)$ is a compact k -particle operator. Propositions 5.10 and 5.12 at the end of this chapter show that $V(x) \frac{1}{1 + \varepsilon \sqrt{1+h}}$ is a compact one-particle operator under suitable assumptions about the magnetic vector potential A . In particular, a magnetic vector potential A that satisfies assumption **(A)** meets the conditions of Proposition 5.10. Lemma 5.15 at the end of this chapter then implies that (5.44) is a compact $(k+1)$ -particle operator on $L^2(\mathbb{R}^{3(k+1)})$. This completes the different approach to showing the vanishing of the term (5.33) in the limit $N \rightarrow \infty$.

Step 3: Uniqueness

In order to finish the proof of Theorem 5.1, we still have to prove the uniqueness of the solution to the infinite hierarchy (5.3). This follows from the next slightly more general result.

Proposition 5.8. Fix $\Gamma_{\infty,0}^{(k)} = \{\gamma_{\infty,0}^{(k)}\}_{k \in \mathbb{N}} \in \bigoplus_{k \in \mathbb{N}} \mathcal{L}_k^1$. Then there exists at most one solution $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \in \mathbb{N}} \in \bigoplus_{k \in \mathbb{N}} C([0, T]; \mathcal{L}_k^1)$ to the infinite hierarchy (4.5) such that $\gamma_{\infty,t=0}^{(k)} = \gamma_{\infty,0}^{(k)}$ and $\operatorname{tr} |\gamma_{\infty,t}^{(k)}| \leq 1$ for all $k \in \mathbb{N}$ and all $t \in [0, T]$.

Proof. Suppose that $\{\gamma_{\infty,1,t}^{(k)}\}_{k \in \mathbb{N}}$ and $\{\gamma_{\infty,2,t}^{(k)}\}_{k \in \mathbb{N}}$ are two solutions of (4.5) with the same initial data $\{\gamma_{\infty,0}^{(k)}\}_{k \in \mathbb{N}}$, such that $\operatorname{tr} |\gamma_{\infty,i,t}^{(k)}| \leq 1$, for all $k \in \mathbb{N}$, $t \in [0, T]$, and for $i = 1, 2$. Then

we can expand the integral equations for $\gamma_{\infty,1,t}^{(k)}$ and $\gamma_{\infty,2,t}^{(k)}$ into the Duhamel series (4.12). It follows that

$$\mathrm{tr} \left| \gamma_{\infty,1,t}^{(k)} - \gamma_{\infty,2,t}^{(k)} \right| \leq \int_0^t ds_1 \cdots \int_0^{s_{n-1}} ds_n \mathrm{tr} \left| \mathcal{U}^{(k)}(t - s_1) B^{(k)} \cdots B^{(k+n-1)} (\gamma_{\infty,1,s_n}^{(k+n)} - \gamma_{\infty,2,s_n}^{(k+n)}) \right|. \quad (5.45)$$

Applying recursively the bounds (4.14) and (4.16), we obtain

$$\mathrm{tr} \left| \gamma_{\infty,1,t}^{(k)} - \gamma_{\infty,2,t}^{(k)} \right| \leq \frac{(k+n-1)!}{(k-1)!n!} (2\|V\|t)^n \leq 2^k (4\|V\|t)^n \quad (5.46)$$

and thus, for $0 < t < \frac{1}{8\|V\|}$,

$$\mathrm{tr} \left| \gamma_{\infty,1,t}^{(k)} - \gamma_{\infty,2,t}^{(k)} \right| \leq 2^{k-n}. \quad (5.47)$$

Since the left-hand side of (5.47) is independent of $n \in \mathbb{N}$, it has to vanish. This proves uniqueness for short times. Iterating the same argument, we obtain uniqueness for all times. \square

Putting things together:

We have now established that the sequence $(\Gamma_{N,t})_{N \in \mathbb{N}}$ is precompact with respect to the topology τ_{prod} and that all its limit points are given by the unique solution $\Gamma_{\infty,t} = \{|\varphi_t\rangle\langle\varphi_t|^{\otimes k}\}_{k \in \mathbb{N}}$ to the infinite hierarchy (5.3).

This implies that the sequence $\{\Gamma_{N,t}\}_{N \in \mathbb{N}}$ actually converges to $\Gamma_{\infty,t} = \{|\varphi_t\rangle\langle\varphi_t|^{\otimes k}\}_{k \in \mathbb{N}}$ with respect to the weak topology τ_{prod} . In particular, it yields the result that for every fixed $k \in \mathbb{N}$ and every fixed $t \in \mathbb{R}$,

$$\lim_{N \rightarrow \infty} \mathrm{tr} J^{(k)}(\gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k}) = 0 \quad (5.48)$$

for all compact operators $J^{(k)} \in \mathcal{K}_k$. Taking $\tilde{J}^{(k)} = |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \in \mathcal{K}_k$, we have

$$0 = \lim_{N \rightarrow \infty} \tilde{J}^{(k)}(\gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k}) = \lim_{N \rightarrow \infty} \langle \varphi_t^{\otimes k}, \gamma_{N,t}^{(k)} \varphi_t^{\otimes k} \rangle - 1. \quad (5.49)$$

Finally, by the relation (2.16), we obtain for every fixed $k \in \mathbb{N}$ and every fixed $t \in \mathbb{R}$, the strong trace norm convergence

$$\lim_{N \rightarrow \infty} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right| = 0. \quad (5.50)$$

\square

Remark 5.9. In this chapter we have adapted the compactness argument for non-relativistic mean-field systems without magnetic fields to the case of systems with external magnetic fields. This required several non-trivial changes. In particular, the proofs of Propositions 5.3 and 5.6 had to be modified significantly to account for an external magnetic field.

We pursued two different approaches to the proof of Proposition 5.6. The idea of the second approach was outlined in Remark 5.7. The main ingredients of this second approach are given below in Propositions 5.10, 5.12 and in Lemma 5.15.

Proposition 5.10. *Let $A \in L^2_{loc}(\mathbb{R}^3; \mathbb{R}^3)$ be such that $(-i\nabla + A)^2$ is self-adjoint on $L^2(\mathbb{R}^3)$ and let $V \in L^\infty(\mathbb{R}^3)$ such that $V(x) \rightarrow 0$ as $|x| \rightarrow \infty$. Then for every $\varepsilon > 0$, the operator*

$$V(x) \frac{1}{1 + \varepsilon \sqrt{1 + (-i\nabla + A)^2}} : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3) \quad (5.51)$$

is compact.

Proof. Let h denote $(-i\nabla + A)^2$ and fix an arbitrary $\varepsilon > 0$. We have

$$V(x) \frac{1}{1 + \varepsilon \sqrt{1 + h}} = \left(V(x) \frac{1}{1 + \varepsilon \sqrt{h}} \right) \left((1 + \varepsilon \sqrt{h}) \frac{1}{1 + \varepsilon \sqrt{1 + h}} \right). \quad (5.52)$$

By functional calculus the operator in the second parentheses is bounded. Suppose the operator in the first parentheses is compact, then the operator on the left-hand side is also compact. It is therefore enough to show the compactness of $V(x) \frac{1}{1 + \varepsilon \sqrt{h}}$.

To this end we will make use of the following result by B. Russo and J. Fournier on trace ideal properties of integral operators. Here $\mathcal{L}^p(L^2(\mathbb{R}^3))$ denotes the p -th trace ideal over $L^2(\mathbb{R}^3)$ with norm $\|\cdot\|_{\mathcal{L}^p}$.

Lemma 5.11. *For a measurable function $k : \mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{C}$ and $1 \leq p, q < \infty$ define*

$$\|k\|_{p,q} = \left(\int \left(\int |k(x,y)|^p dx \right)^{q/p} dy \right)^{1/q}. \quad (5.53)$$

Let $T : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$ be an integral operator with kernel k and $2 \leq p < \infty$. Then

$$\|T\|_{\mathcal{L}^p} \leq (\|k\|_{p',p} \|k^*\|_{p',p})^{1/2}, \quad (5.54)$$

where $k^*(x,y) := \overline{k(y,x)}$ and $\frac{1}{p} + \frac{1}{p'} = 1$. In particular, if T has kernel $k(x,y) = f(x)g(x-y)$, using Young's inequality, this implies

$$\|T\|_{\mathcal{L}^p} \leq (\|k\|_{p',p} \|k^*\|_{p',p})^{1/2} \leq \|f\|_p \|g\|_{p'}. \quad (5.55)$$

Proof. See the remarks to Corollary 2, in particular equation (10), in [16]. Also compare with equation (4.9) in the remark to the proof of Theorem 4.1 in [36]. \square

Set $V_n(x) := \chi_{\{|x| \leq n\}}(x)V(x)$ for $n \in \mathbb{N}$ and define the operators

$$\tilde{T}_n := \frac{1}{\varepsilon} V_n(x) \frac{1}{\frac{1}{\varepsilon} + \sqrt{h}} \quad \text{and} \quad T_n := \frac{1}{\varepsilon} V_n(x) \frac{1}{\frac{1}{\varepsilon} + \sqrt{-\Delta}}. \quad (5.56)$$

Denote by $\tilde{T}_n(x,y)$ and $T_n(x,y)$ the integral kernels of \tilde{T}_n and, respectively, of T_n . By the relativistic diamagnetic inequality (8.13), which requires $A \in L^2_{loc}(\mathbb{R}^3; \mathbb{R}^3)$, we have for any $e > 0$ that for almost every $x, y \in \mathbb{R}^3$:

$$\left| \frac{1}{e + \sqrt{h}}(x,y) \right| \leq \frac{1}{e + \sqrt{-\Delta}}(x,y). \quad (5.57)$$

Thus, for almost every $x, y \in \mathbb{R}^3$:

$$|\tilde{T}_n(x, y)| \leq \frac{1}{\varepsilon} |V_n(x)| \left| \frac{1}{\frac{1}{\varepsilon} + \sqrt{h}}(x, y) \right| \leq \frac{1}{\varepsilon} |V_n(x)| \frac{1}{\frac{1}{\varepsilon} + \sqrt{-\Delta}}(x, y) = |T_n(x, y)|. \quad (5.58)$$

The kernel $\frac{1}{\frac{1}{\varepsilon} + \sqrt{-\Delta}}(x, y)$ is of the type $g(x - y)$ for some function $g : \mathbb{R}^3 \rightarrow \mathbb{R}$ as shown below. Lemma 5.11 then yields

$$\|\tilde{T}_n\|_{\mathcal{L}^p} \leq (\|\tilde{T}_n(x, y)\|_{p', p} \|\tilde{T}_n^*(x, y)\|_{p', p})^{1/2} \leq (\|T_n(x, y)\|_{p', p} \|T_n^*(x, y)\|_{p', p})^{1/2} \leq \frac{1}{\varepsilon} \|V_n\|_p \|g\|_{p'} \quad (5.59)$$

for any $2 \leq p < \infty$. Below we will show that $g \in L^{p'}(\mathbb{R}^3)$ for any $1 < p' < \frac{3}{2}$. Hence \tilde{T}_n is in $\mathcal{L}^p(L^2(\mathbb{R}^3))$, and in particular compact, for every $n \in \mathbb{N}$. By the definition of V_n and the assumption that V vanishes at infinity, we have $\left\| V(x) \frac{1}{1 + \varepsilon \sqrt{h}} - \tilde{T}_n \right\| \rightarrow 0$ in operator norm as $n \rightarrow \infty$. Hence, the operator $V(x) \frac{1}{1 + \varepsilon \sqrt{h}}$ is compact.

It remains to verify the above mentioned properties of the integral kernel of $\frac{1}{\frac{1}{\varepsilon} + \sqrt{-\Delta}}$. By functional calculus we have

$$\frac{1}{\frac{1}{\varepsilon} + \sqrt{-\Delta}} = \int_0^\infty dt e^{-t(\frac{1}{\varepsilon} + \sqrt{-\Delta})} = \int_0^\infty dt e^{-\frac{1}{\varepsilon}t} e^{-t\sqrt{-\Delta}}. \quad (5.60)$$

Using the explicit representation of the relativistic heat kernel in three dimensions (8.14),

$$e^{-t\sqrt{-\Delta}}(x, y) = \frac{1}{\pi^2} \frac{t}{(t^2 + |x - y|^2)^2} \quad \text{for } x, y \in \mathbb{R}^3, \quad (5.61)$$

we can compute the integral kernel of $\frac{1}{\frac{1}{\varepsilon} + \sqrt{-\Delta}}$: For any $\psi \in L^2(\mathbb{R}^3)$ we have

$$\begin{aligned} \left(\frac{1}{\frac{1}{\varepsilon} + \sqrt{-\Delta}} \psi \right) (x) &= \int_0^\infty dt e^{-\frac{1}{\varepsilon}t} e^{-t\sqrt{-\Delta}} \psi(x) \\ &= \int_0^\infty dt e^{-\frac{1}{\varepsilon}t} \int_{\mathbb{R}^3} dy \frac{1}{\pi^2} \frac{t}{(t^2 + |x - y|^2)^2} \psi(y) \\ &= \int_{\mathbb{R}^3} dy \frac{1}{\pi^2} \int_0^\infty dt \frac{te^{-\frac{1}{\varepsilon}t}}{(t^2 + |x - y|^2)^2} \psi(y) \\ &\equiv \int_{\mathbb{R}^3} dy g(x - y) \psi(y). \end{aligned} \quad (5.62)$$

Thus

$$\frac{1}{\frac{1}{\varepsilon} + \sqrt{-\Delta}}(x, y) \equiv g(x - y) = \frac{1}{\pi^2} \int_0^\infty dt \frac{te^{-\frac{1}{\varepsilon}t}}{(t^2 + |x - y|^2)^2}. \quad (5.63)$$

Now for $q \geq 1$:

$$\begin{aligned}
& \int_{\mathbb{R}^3} dx |g(x)|^q \\
&= \int_{\mathbb{R}^3} dx \left| \frac{1}{\pi^2} \int_0^\infty dt \frac{te^{-\frac{1}{\varepsilon}t}}{(t^2 + |x|^2)^2} \right|^q \\
&= C \int_0^\infty dr r^2 \left| \int_0^\infty dt \frac{te^{-\frac{1}{\varepsilon}t}}{(t^2 + r^2)^2} \right|^q \\
&= C \int_0^\infty dr r^{2-2q} \left| \int_0^\infty ds \frac{se^{-\frac{1}{\varepsilon}rs}}{(1+s^2)^2} \right|^q \\
&= C \int_0^1 dr r^{2-2q} \left| \int_0^\infty ds \frac{se^{-\frac{1}{\varepsilon}rs}}{(1+s^2)^2} \right|^q + C \int_1^\infty dr r^{2-2q} \left| \int_0^\infty ds \left(-\frac{\varepsilon}{r}\right) \left(\frac{\partial}{\partial s} e^{-\frac{1}{\varepsilon}rs}\right) \frac{s}{(1+s^2)^2} \right|^q \\
&\leq C \int_0^1 dr r^{2-2q} \left| \int_0^\infty ds \frac{s}{(1+s^2)^2} \right|^q + C \int_1^\infty dr r^{2-3q} \left| \int_0^\infty ds \varepsilon \left| \frac{\partial}{\partial s} \left(\frac{s}{(1+s^2)^2} \right) \right| \right|^q \\
&= Cc_1^q \int_0^1 dr r^{2-2q} + Cc_2^q \int_1^\infty dr r^{2-3q},
\end{aligned} \tag{5.64}$$

where we performed an integration by parts in the penultimate step. Since $c_1 = \int_0^\infty ds \frac{s}{(1+s^2)^2} < \infty$ and $c_2 = \int_0^\infty ds \varepsilon \left| \frac{\partial}{\partial s} \left(\frac{s}{(1+s^2)^2} \right) \right| < \infty$, the expression in the last line is finite for any $1 < q < \frac{3}{2}$. Hence, $g \in L^q(\mathbb{R}^3)$ for any $1 < q < \frac{3}{2}$, which completes the proof. \square

We found an alternative proof for the compactness of the operator (5.51) under more restrictive conditions applying to the magnetic vector potential A . It is stated in Proposition 5.12 below. However, notice that not all vector potentials A satisfying the assumption **(A)** fulfil the conditions of Proposition 5.12 below.

For the magnetic one-particle operator h we introduce the shorthand notation

$$h = (-i\nabla + A)^2 = -\Delta - 2iA \cdot \nabla - i(\nabla \cdot A) + A^2 \equiv S + T, \tag{5.65}$$

where $S \equiv -\Delta$ and $T \equiv -2iA \cdot \nabla - i(\nabla \cdot A) + A^2$. The idea of the proof of Proposition 5.12 is of perturbative nature. We will treat T as a perturbation of the operator $S \equiv -\Delta$, which is self-adjoint on $L^2(\mathbb{R}^3)$. In this way we will reduce the proof of the compactness of the operator (5.51) to the unperturbed case, i.e. the proof of the compactness of the operator $V(x) \frac{1}{1+\varepsilon\sqrt{1-\Delta}}$. The latter follows from Theorem 8.13.

Proposition 5.12. *Let $V \in L^\infty(\mathbb{R}^3)$ such that $V(x) \rightarrow 0$ as $|x| \rightarrow \infty$. Suppose that the magnetic vector potential $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is such that T is S -bounded with relative bound $\tilde{a} < 1$, i.e. $D(T) \supseteq D(S)$ and there exists some $\tilde{b} > 0$ such that*

$$\|T\varphi\| \leq \tilde{a}\|S\varphi\| + \tilde{b}\|\varphi\| \tag{5.66}$$

holds for all $\varphi \in D(S)$. Then for every $\varepsilon > 0$, the operator

$$V(x) \frac{1}{1 + \varepsilon \sqrt{1 + (-i\nabla + A)^2}} : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3) \quad (5.67)$$

is compact.

Proof. Under the given assumptions, the Kato-Rellich Theorem 8.12 implies that $h = S + T$ is self-adjoint on the domain of S . To simplify the notation, we shall only prove the assertion for the case $\varepsilon = 1$. For other values of ε , obvious modifications of the proof give the result. Consider the splitting

$$\begin{aligned} V(x) \frac{1}{1 + \sqrt{1 + h}} &\equiv V(x) \frac{1}{1 + \sqrt{1 + S + T}} \\ &= \left(V(x) \frac{1}{1 + \sqrt{1 + S}} \right) \left((1 + \sqrt{1 + S}) \frac{1}{1 + \sqrt{1 + S + T}} \right). \end{aligned} \quad (5.68)$$

The operator in the first parentheses is compact by the “ $f(x)g(-i\nabla)$ – Theorem” 8.13. In order to prove the compactness of the operator on the left-hand side of (5.68), it therefore suffices to show that the operator in the second parentheses is bounded. By functional calculus, we can estimate as follows:

$$\begin{aligned} \left\| (1 + \sqrt{1 + S}) \frac{1}{1 + \sqrt{1 + S + T}} \right\| &\leq \left\| \frac{1}{1 + \sqrt{1 + S + T}} \right\| + \left\| \sqrt{1 + S} \frac{1}{1 + \sqrt{1 + S + T}} \right\| \\ &\leq 1 + \left\| \sqrt{1 + S} \frac{1}{\sqrt{1 + S + T}} \right\| \left\| \sqrt{1 + S + T} \frac{1}{1 + \sqrt{1 + S + T}} \right\| \\ &\leq 1 + \left\| \sqrt{1 + S} \frac{1}{\sqrt{1 + S + T}} \right\|. \end{aligned} \quad (5.69)$$

Using the identity $\|\hat{O}\|^2 = \|\hat{O}^* \hat{O}\|$ for the operator norm of a self-adjoint operator \hat{O} , we obtain

$$\begin{aligned} \left\| \sqrt{1 + S} \frac{1}{\sqrt{1 + S + T}} \right\|^2 &= \left\| \frac{1}{\sqrt{1 + S + T}} (1 + S) \frac{1}{\sqrt{1 + S + T}} \right\| \\ &\leq \left\| \frac{1}{1 + S + T} \right\| + \left\| \frac{1}{\sqrt{1 + S + T}} S \frac{1}{\sqrt{1 + S + T}} \right\| \\ &\leq 1 + \left\| (1 + \hat{A})^{-\frac{1}{2}} \hat{B} (1 + \hat{A})^{-\frac{1}{2}} \right\|, \end{aligned} \quad (5.70)$$

where we use the notation $\hat{B} \equiv S$ and $\hat{A} \equiv S + T$. By our initial assumptions on T , $\hat{A} \equiv S + T = (-i\nabla + A)^2$ is a positive self-adjoint operator and $\hat{B} \equiv S = -\Delta$ is self-adjoint. Moreover, for every $\varphi \in D(S) = D(S + T)$,

$$\|S\varphi\| \leq \|(S + T)\varphi\| + \|(-T)\varphi\| \leq \|(S + T)\varphi\| + \tilde{a}\|S\varphi\| + \tilde{b}\|\varphi\|. \quad (5.71)$$

Hence

$$\|S\varphi\| \leq \frac{1}{1 - \tilde{a}} \|(S + T)\varphi\| + \frac{\tilde{b}}{1 - \tilde{a}} \|\varphi\|, \quad (5.72)$$

so \hat{B} is \hat{A} -bounded with relative bound $a = \frac{1}{1 - \tilde{a}}$. Lemma 5.13 below now yields a bound on $\left\| (1 + \hat{A})^{-\frac{1}{2}} \hat{B} (1 + \hat{A})^{-\frac{1}{2}} \right\|$, which completes the proof of Proposition 5.12. \square

Lemma 5.13. *If \hat{A} is a positive self-adjoint operator and \hat{B} is a self-adjoint operator, which is \hat{A} -bounded with relative bound a and corresponding constant b , then*

$$\left\| (1 + \hat{A})^{-\frac{1}{2}} \hat{B} (1 + \hat{A})^{-\frac{1}{2}} \right\| \leq a + b. \quad (5.73)$$

Proof. See the proof of Theorem X.18 in [31]. \square

Remark 5.14. Note that a linear magnetic vector potential A , which generates a constant magnetic field B , does not satisfy the assumptions of Proposition 5.12. However, an appropriately chosen magnetic vector potential A of a smooth, compactly supported magnetic field B , does meet the conditions of Proposition 5.12.

Moreover, by Theorem X.22 in [31], a magnetic vector potential $A \in L^4(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with $\nabla \cdot A \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ satisfies the conditions of Proposition 5.12.

Lemma 5.15. *Let $J^{(k)}$ be a compact operator on $L^2(\mathbb{R}^{3k})$ and let $\varepsilon > 0$. Suppose $V \in L^\infty(\mathbb{R}^3)$ with $V(x) \rightarrow 0$ as $|x| \rightarrow \infty$. Assume that the magnetic vector potential $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is such that the one-particle operator $V(x) \frac{1}{1 + \varepsilon \sqrt{1 + h}}$ is compact on $L^2(\mathbb{R}^3)$, where $h = (-i\nabla + A)^2$. Then the operator*

$$J^{(k)} V(x_1 - x_{k+1}) \frac{1}{1 + \varepsilon \sqrt{1 + h_{k+1}}} \quad (5.74)$$

is compact on $L^2(\mathbb{R}^{3(k+1)})$.

Proof. It is enough to show the compactness of the operator

$$K \equiv J V(x - y) \frac{1}{1 + \varepsilon \sqrt{1 + h}}, \quad (5.75)$$

on $L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$, where J is a compact one-particle operator on $L^2(\mathbb{R}^3)$ and h is a magnetic operator in the variable y . To this end we will use the fact that the set of compact operators is closed under the operator norm. In order to prove that the operator K is compact, it is therefore enough to approximate it with an operator norm convergent sequence of compact operators. Moreover, it is a fact that the finite rank operators are dense in the set of compact operators on $L^2(\mathbb{R}^3)$ (see e.g. Theorem VI.12 and Theorem VI.13 in [32]).

Since V is bounded and vanishes at infinity, it can be approximated by a sequence of compactly supported bounded functions V_n such that $\|V - V_n\|_\infty \rightarrow 0$ as $n \rightarrow \infty$. Since

$$\left\| J V(x - y) \frac{1}{1 + \varepsilon \sqrt{1 + h}} - J V_n(x - y) \frac{1}{1 + \varepsilon \sqrt{1 + h}} \right\| \leq \|J\| \|V - V_n\| \left\| \frac{1}{1 + \varepsilon \sqrt{1 + h}} \right\| \rightarrow 0 \quad (5.76)$$

as $n \rightarrow \infty$, we can from now on assume V to be compactly supported and bounded.

Moreover, since J is compact, it can be approximated by a sequence $(J_n)_n$ of finite rank operators such that $\|J - J_n\| \rightarrow 0$ as $n \rightarrow \infty$. We have

$$\left\| J V(x - y) \frac{1}{1 + \varepsilon \sqrt{1 + h}} - J_n V(x - y) \frac{1}{1 + \varepsilon \sqrt{1 + h}} \right\| \leq \|J - J_n\| \|V\| \left\| \frac{1}{1 + \varepsilon \sqrt{1 + h}} \right\| \rightarrow 0 \quad (5.77)$$

as $n \rightarrow \infty$. It is therefore sufficient to show that $J_n V(x-y) \frac{1}{1+\varepsilon\sqrt{1+h}}$ is compact. By linearity, we can assume that J_n is a rank one operator, i.e. $J_n = |\psi\rangle\langle\phi|$ for some $\psi, \phi \in L^2(\mathbb{R}^3)$. By another approximation argument, we can assume that ψ and ϕ actually have compact support. The kernel of the operator $T \equiv J_n V(x-y) \frac{1}{1+\varepsilon\sqrt{1+h}}$ is then

$$T(x, y; x', y') = \psi(x) \overline{\phi(x')} V(x' - y) \frac{1}{1 + \varepsilon\sqrt{1+h}}(y; y'). \quad (5.78)$$

Since ϕ and V are both compactly supported, $\overline{\phi(x')} V(x' - y)$ vanishes for $|y| \geq R$ for some large enough $R > 0$. We are therefore free to insert the characteristic function $\chi_R(y) = \mathbb{1}_{\{|y| \leq R\}}$:

$$T(x, y; x', y') = \psi(x) \overline{\phi(x')} V(x' - y) \chi_R(y) \frac{1}{1 + \varepsilon\sqrt{1+h}}(y; y'). \quad (5.79)$$

The characteristic function χ_R is obviously bounded and compactly supported. By assumption, $\chi_R \frac{1}{1+\varepsilon\sqrt{1+h}}$ is then a compact operator on $L^2(\mathbb{R}^3)$. With the same approximation argument as above, we can assume that it is a rank one operator $|f\rangle\langle g|$ for some $f, g \in L^2(\mathbb{R}^3)$. So T has kernel

$$T(x, y; x', y') = \psi(x) \overline{\phi(x')} V(x' - y) f(y) \overline{g(y')} \quad (5.80)$$

and its Hilbert-Schmidt norm

$$\int dx dx' dy dy' |T(x, y; x', y')|^2 = \int dx dx' dy dy' |\psi(x)|^2 |\phi(x')|^2 |V(x' - y)|^2 |f(y)|^2 |g(y')|^2 \quad (5.81)$$

is finite, because V is bounded and $\psi, \phi, f, g \in L^2(\mathbb{R}^3)$. Hence, T is a Hilbert-Schmidt operator and in particular compact, which completes the proof. \square

Remark 5.16. We would like to thank Prof. Erdős for showing us the proof of Lemma 5.15.

Chapter 6

Projections method

In the first part of this chapter we will explain the approach by Knowles and Pickl to derive effective evolution equations from quantum dynamics for mean-field systems for arbitrary dimension d . In the second part we will apply their method to mean-field systems with magnetic fields. This latter part only treats $d = 3$ dimensions.

6.1 Outline of the method

We shall consider interaction potentials $V \in L^2(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$. The analysis of [24] can be extended to more singular interaction potentials. This requires further technicalities and assumptions about the initial state that are more stringent. In order to understand the main idea of the method we will therefore restrict ourselves to the above class of potentials, which includes the important case of Coulomb interactions for $d = 3$. The exposition in this section largely follows that in [24].

The method relies on controlling the quantity

$$\alpha_N(t) = E_N^{(1)}(t) = 1 - \langle \varphi_t, \gamma_{N,t}^{(1)} \varphi_t \rangle \quad (6.1)$$

over its evolution in time. We saw in Chapter 2 that $E_N^{(1)}(t)$ in turn controls the trace norm distance of all higher k -particle marginals $\gamma_{N,t}^{(k)}$ from the corresponding factorised solutions of the infinite hierarchy, $|\varphi_t\rangle\langle\varphi_t|^{\otimes k}$. We will compute the derivative of $\alpha_N(t)$ and show that it satisfies an estimate of the form

$$\dot{\alpha}_N(t) \leq A_N(t) + B_N(t)\alpha_N(t). \quad (6.2)$$

Then, by Grönwall's Lemma,

$$\alpha_N(t) \leq \left(\alpha_N(0) + \int_0^t ds A_N(s) \right) e^{\int_0^t ds B_N(s)}. \quad (6.3)$$

The scaling of A_N and B_N with N will then give the appropriate behaviour of α_N as $N \rightarrow \infty$.

To simplify the notation in what follows, we rewrite the Hamiltonian (1.7) as

$$H_N = \sum_{j=1}^N h_j + \frac{1}{N} \sum_{i<j}^N V_{ij} =: H_N^0 + H_N^V, \quad (6.4)$$

where $V_{ij} := V(x_i - x_j)$.

We make the following assumptions:

(A1) The one-particle Hamiltonian h is self-adjoint and bounded from below. Without loss of generality we assume that $h \geq 0$. We define the Hilbert space $X_N = \mathcal{Q}(H_N^0)$ as the form domain of H_N^0 with norm

$$\|\psi\|_{X_N} := \|(\mathbf{1} + H_N^0)^{1/2}\psi\|_2. \quad (6.5)$$

(A2) The Hamiltonian H_N is self-adjoint and bounded from below. We also assume that $\mathcal{Q}(H_N) \subset X_N$, where $\mathcal{Q}(H_N)$ is the form domain of H_N .

(A3) The interaction potential V is a real and even function satisfying $V \in L^{p_1} + L^{p_2}$, where $2 \leq p_1 \leq p_2 \leq \infty$.

(A4) The solution φ_t to the Hartree equation (1.11) with initial data $\varphi \in X_1 \cap L^{q_1}$ satisfies

$$\varphi_t \in C(\mathbb{R}; X_1 \cap L^{q_1}) \cap C^1(\mathbb{R}; X_1^*), \quad (6.6)$$

where $2 \leq q_2 \leq q_1 \leq \infty$ are defined by

$$\frac{1}{2} = \frac{1}{p_i} + \frac{1}{q_i}, \quad i = 1, 2. \quad (6.7)$$

Here X_1^* denotes the dual space of X_1 , i.e. the closure of L^2 under the norm $\|\varphi\|_{X_1^*} := \|(\mathbf{1} + h)^{-1/2}\varphi\|_2$.

We can now state the main result.

Theorem 6.1 (Knowles-Pickl, [24]). *Let $\psi_N \in \mathcal{Q}(H_N)$ satisfy $\|\psi_N\|_2 = 1$, and $\varphi \in X_1 \cap L^{q_1}$ satisfy $\|\varphi\|_2 = 1$. Assume that the assumptions (A1) - (A4) hold. Then*

$$\alpha_N(t) \leq \left(\alpha_N(0) + \frac{1}{N} \right) e^{\phi(t)}, \quad (6.8)$$

where

$$\phi(t) := 32\|V\|_{L^{p_1}+L^{p_2}} \int_0^t ds (\|\varphi(s)\|_{q_1} + \|\varphi(s)\|_{q_2}). \quad (6.9)$$

Using the results of Chapter 2 we obtain

Corollary 6.2. *Let the sequence $\psi_N \in \mathcal{Q}(H_N)$, $N \in \mathbb{N}$, satisfy the assumptions of Theorem 6.1 as well as*

$$E_N^{(1)}(0) \leq \frac{C}{N}. \quad (6.10)$$

for some $C > 0$. Then we have

$$E_N^{(k)}(t) \leq (C+1) \frac{k}{N} e^{\phi(t)}, \quad R_N^{(k)}(t) \leq 2\sqrt{C+1} \sqrt{\frac{k}{N}} e^{\phi(t)/2}. \quad (6.11)$$

Remark 6.3. For an initially factorised state $\psi_N = \varphi^{\otimes N}$, we have trivially $E_N^{(1)}(0) = 0$, and Corollary 6.2 reads

$$E_N^{(k)}(t) \leq \frac{k}{N} e^{\phi(t)}, \quad R_N^{(k)}(t) \leq 2\sqrt{\frac{k}{N}} e^{\phi(t)/2}. \quad (6.12)$$

This implies that for every fixed $k \in \mathbb{N}$ and every fixed $t \in \mathbb{R}$:

$$\lim_{N \rightarrow \infty} \operatorname{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right| = 0. \quad (6.13)$$

Remark 6.4. In some cases it is convenient to modify the assumptions as follows. Replace (A3) and (A4) with

(A3') The interaction potential V is a real and even function satisfying

$$\|V^2 * |\varphi|^2\|_\infty \leq K \|\varphi\|_{X_1}^2 \quad (6.14)$$

for some constant $K > 0$. Without loss of generality we assume that $K \geq 1$.

(A4') The solution φ_t of (3.3) satisfies

$$\varphi_t \in C(\mathbb{R}; X_1) \cap C^1(\mathbb{R}; X_1^*). \quad (6.15)$$

Then Theorem 6.1 and Corollary 6.2 hold with

$$\phi(t) = 32K \int_0^t ds \|\varphi_s\|_{X_1}^2. \quad (6.16)$$

The proof even simplifies. One replaces (6.54) with (6.14), and (6.43) with

$$\|V * |\varphi|^2\|_\infty \leq 2K \|\varphi\|_{X_1}^2, \quad (6.17)$$

which follows directly from (6.14).

Proof of Theorem 6.1. We introduce the projection operators

$$p(t) := |\varphi_t\rangle\langle\varphi_t| \quad \text{and} \quad q(t) := \mathbb{1} - p(t), \quad (6.18)$$

where $\mathbb{1}$ is the identity on $L^2(\mathbb{R}^d)$. For $j \in \{1, \dots, N\}$ we use the notation

$$p_j(t) = \mathbb{1}_1 \otimes \dots \otimes \mathbb{1}_{j-1} \otimes p(t) \otimes \mathbb{1}_{j+1} \otimes \dots \otimes \mathbb{1}_N \quad (6.19)$$

and $q_j(t) = \mathbb{1}_{L^2(\mathbb{R}^{Nd})} - p_j(t)$. Next, define

$$P_k(t) := \sum_{\substack{a \in \{0,1\}^N \\ \sum_j a_j = k}} \prod_{j=1}^N p_j(t)^{1-a_j} q_j(t)^{a_j} \quad (6.20)$$

and set $P_k(t) = 0$ if $k \notin \{0, 1, \dots, N\}$. $P_k(t)$ has the following properties:

- (i) $P_k(t)$ is an orthogonal projection,

- (ii) $P_k(t)P_l(t) = \delta_{kl}P_k(t)$,
 (iii) $\sum_{k=0}^N P_k(t) = \mathbf{1}_{L^2(\mathbb{R}^{Nd})}$.

Moreover, for any function $f : \mathbb{Z} \rightarrow \mathbb{C}$ with $\text{supp}(f) \subseteq \{0, 1, \dots, N\}$ we define the operator

$$\hat{f}(t) := \sum_{k=0}^N f(k)P_k(t). \quad (6.21)$$

It follows that

$$\hat{f}(t)\hat{g}(t) = \widehat{fg}(t), \quad (6.22)$$

and that $\hat{f}(t)$ commutes with $p_j(t)$ and $P_k(t)$. We will often use the functions

$$m(k) := \frac{k}{N}, \quad n(k) := \sqrt{\frac{k}{N}} \quad \text{for } k \in \{0, 1, \dots, N\} \quad (6.23)$$

and $m(k) = n(k) := 0$ otherwise. From the definition of $q_j(t)$ and $P_k(t)$ we obtain

$$\frac{1}{N} \sum_{j=1}^N q_j(t) = \frac{1}{N} \sum_{j=1}^N \sum_{k=0}^N q_j(t)P_k(t) = \frac{1}{N} \sum_{k=1}^N kP_k(t) = \hat{m}(t). \quad (6.24)$$

By the symmetry of the wave function $\psi_{N,t}$ and the definition of partial trace, this allows us to rewrite $\alpha_N(t)$ as

$$\begin{aligned} \alpha_N(t) &= 1 - \langle \varphi_t, \gamma_{N,t}^{(1)} \varphi_t \rangle = \langle \psi_{N,t}, q_1(t) \psi_{N,t} \rangle = \langle \psi_{N,t}, \frac{1}{N} \sum_{j=1}^N q_j(t) \psi_{N,t} \rangle \\ &= \sum_{k=1}^N \frac{k}{N} \langle \psi_{N,t}, P_k(t) \psi_{N,t} \rangle = \langle \psi_{N,t}, \hat{m}(t) \psi_{N,t} \rangle. \end{aligned} \quad (6.25)$$

Let us emphasise what $\alpha_N(t)$ does. The part of $\psi_{N,t}$ where k of the N particles are not in the state φ_t (i.e. $\langle \psi_{N,t}, P_k(t) \psi_{N,t} \rangle$) is given the weight $\frac{k}{N}$. Thus, intuitively, $\alpha_N(t)$ counts the relative number of particles which are not in the state φ_t .

Now we introduce the shift operation τ_n , $n \in \mathbb{Z}$, defined on functions f through

$$(\tau_n f)(k) := f(k+n). \quad (6.26)$$

We will use the following lemma several times in the main part of the proof of Theorem 6.1.

Lemma 6.5. *Let A be an operator acting on $L^2(\mathbb{R}^d) \otimes L^2(\mathbb{R}^d)$ and define $A_{1,2} := A \otimes \mathbf{1}_3 \otimes \dots \otimes \mathbf{1}_N$. Let Q_i , $i = 1, 2$, be two operators of the form*

$$Q_i = \#_1 \#_2, \quad (6.27)$$

where $\#$ denotes either $p(t)$ or $q(t)$. Then

$$Q_1 A_{1,2} \hat{f}(t) Q_2 = Q_1 \widehat{\tau_n f}(t) A_{1,2} Q_2, \quad (6.28)$$

where $n = n_2 - n_1$ and n_i is the number of factors $q(t)$ in Q_i (n_i can be either 0, 1 or 2).

Proof. Define

$$P_k^{(2)}(t) = \sum_{\substack{a \in \{0,1\}^{N-2} \\ \sum_j a_j = k}} \prod_{j=3}^N p_j(t)^{1-a_j} q_j(t)^{a_j}. \quad (6.29)$$

Then

$$\hat{f}(t)Q_i = Q_i\hat{f}(t) = \sum_{k=0}^N f(k)Q_iP_k(t) = \sum_{k=0}^N f(k)Q_iP_{k-n_i}^{(2)}(t) = \sum_{k=0}^N f(k+n_i)Q_iP_k^{(2)}(t). \quad (6.30)$$

Using the fact that $A_{1,2}$ commutes with $P_k^{(2)}(t)$ we therefore obtain

$$\begin{aligned} Q_1A_{1,2}\hat{f}(t)Q_2 &= \sum_{k=0}^N f(k+n_2)Q_1A_{1,2}P_k^{(2)}(t)Q_2 \\ &= \sum_{k=0}^N f(k+n_2)Q_1P_k^{(2)}(t)A_{1,2}Q_2 \\ &= \sum_{k=0}^N f(k+n_2-n_1)Q_1P_k(t)A_{1,2}Q_2 \\ &= Q_1(\widehat{\tau_n f})(t)A_{1,2}Q_2. \end{aligned} \quad (6.31)$$

□

Estimate of $\dot{\alpha}_N(t)$:

We can now proceed to the main part of the proof and derive a Grönwall - type estimate on $\dot{\alpha}_N(t)$. We use the abbreviations

$$V^{\varphi t} := V * |\varphi_t|^2, \quad H^{\varphi t} := \sum_{j=1}^N h_j + V_j^{\varphi t}. \quad (6.32)$$

Let $\psi \in L^2(\mathbb{R}^{Nd})$. From the assumption (A4) we deduce for $j \in \{1, \dots, N\}$ that

$$\partial_t \langle \psi, p_j(t)\psi \rangle = (-i) \langle \psi, [(h_j + V_j^{\varphi t}), p_j(t)] \psi \rangle = (-i) \langle \psi, [H^{\varphi t}, p_j(t)] \psi \rangle \quad (6.33)$$

using the fact that $[(h_i + V_i^{\varphi t}), p_j(t)] = 0$ for $i \neq j$. We also have

$$\partial_t \langle \psi, q_j(t)\psi \rangle = (-i) \langle \psi, [H^{\varphi t}, q_j(t)] \psi \rangle. \quad (6.34)$$

Thus, using (6.25) and the symmetry of $\psi_{N,t}$, we obtain

$$\begin{aligned}
\dot{\alpha}_N(t) &= \partial_t \langle \psi_{N,t}, \hat{m}(t) \psi_{N,t} \rangle \\
&= i \langle \psi_{N,t}, [H_N, \hat{m}(t)] \psi_{N,t} \rangle - i \langle \psi_{N,t}, [H^{\varphi_t}, q_1(t)] \psi_{N,t} \rangle \\
&= i \langle \psi_{N,t}, [H_N, \hat{m}(t)] \psi_{N,t} \rangle - i \langle \psi_{N,t}, [H^{\varphi_t}, \frac{1}{N} \sum_{j=1}^N q_j(t)] \psi_{N,t} \rangle \\
&= i \langle \psi_{N,t}, [H_N - H^{\varphi_t}, \hat{m}(t)] \psi_{N,t} \rangle \\
&= i \langle \psi_{N,t}, [\frac{1}{N} \sum_{i < j}^N V_{ij} - \sum_{j=1}^N V_j^{\varphi_t}, \hat{m}(t)] \psi_{N,t} \rangle \\
&= \frac{i}{2} \langle \psi_{N,t}, [(N-1)V_{12} - NV_1^{\varphi_t} - NV_2^{\varphi_t}, \hat{m}(t)] \psi_{N,t} \rangle.
\end{aligned} \tag{6.35}$$

Notice that the one-particle operator h drops out of the expression. This is the reason why the method can account for several types of one-particle operators in the same way.

In order to estimate $\dot{\alpha}_N(t)$ we introduce

$$\mathbb{1}_{L^2(\mathbb{R}^{Nd})} = (p_1(t) + q_1(t))(p_2(t) + q_2(t)) \tag{6.36}$$

on both sides of the commutator and expand the expression. Several of the 16 resulting terms vanish because of Lemma 6.5. More precisely, all terms with an equal number of factors $q(t)$ on both sides of the commutator vanish. Only three types remain:

$$\frac{i}{2} \langle \psi_{N,t}, p_1(t)p_2(t) [(N-1)V_{12} - NV_1^{\varphi_t} - NV_2^{\varphi_t}, \hat{m}(t)] q_1(t)p_2(t) \psi_{N,t} \rangle \quad (I)$$

$$\frac{i}{2} \langle \psi_{N,t}, q_1(t)p_2(t) [(N-1)V_{12} - NV_1^{\varphi_t} - NV_2^{\varphi_t}, \hat{m}(t)] q_1(t)q_2(t) \psi_{N,t} \rangle \quad (II)$$

$$\frac{i}{2} \langle \psi_{N,t}, p_1(t)p_2(t) [(N-1)V_{12} - NV_1^{\varphi_t} - NV_2^{\varphi_t}, \hat{m}(t)] q_1(t)q_2(t) \psi_{N,t} \rangle \quad (III).$$

All in all, we have

$$\dot{\alpha}_N(t) = 2(I) + 2(II) + (III) + \text{complex conjugates}. \tag{6.37}$$

It remains to estimate each of the three terms. To this end we use the following heuristics. We control the singularities of V with $p(t)$ by using the regularity of the solution φ_t of the Hartree equation. Factors $q(t)$ give something small of the order $\alpha_N(t)$.

Estimate of (I): Observe first that

$$p_2(t)V_{12}p_2(t) = p_2(t)V_1^{\varphi_t}. \tag{6.38}$$

This can be seen explicitly on the level of kernels. Dropping the irrelevant indices $x_3, y_3, \dots, x_N, y_N$ we have

$$\begin{aligned}
(p_2(t)V_{12}p_2(t))(x_1, x_2; y_1, y_2) &= \int dz \varphi_t(x_2) \overline{\varphi_t(z)} V(x_1 - z) \delta(x_1 - y_1) \varphi_t(z) \overline{\varphi_t(y_2)} \\
&= \delta(x_1 - y_1) \varphi_t(x_2) \overline{\varphi_t(y_2)} \int dz V(x_1 - z) |\varphi_t(z)|^2 \\
&= \delta(x_1 - y_1) \varphi_t(x_2) \overline{\varphi_t(y_2)} (V * |\varphi_t|^2)(x_1) \\
&= (p_2(t)V_1^{\varphi_t})(x_1, x_2; y_1, y_2).
\end{aligned} \tag{6.39}$$

Thus,

$$\begin{aligned}
(I) &= \frac{i}{2} \langle \psi_{N,t}, p_1(t) p_2(t) [(N-1)V_{12} - NV_1^{\varphi_t} - NV_2^{\varphi_t}, \hat{m}(t)] q_1(t) p_2(t) \psi_{N,t} \rangle \\
&= \frac{i}{2} \langle \psi_{N,t}, p_1(t) p_2(t) [(N-1)V_1^{\varphi_t} - NV_1^{\varphi_t}, \hat{m}(t)] q_1(t) p_2(t) \psi_{N,t} \rangle \\
&= -\frac{i}{2} \langle \psi_{N,t}, p_1(t) p_2(t) [V_1^{\varphi_t}, \hat{m}(t)] q_1(t) p_2(t) \psi_{N,t} \rangle \\
&= -\frac{i}{2N} \langle \psi_{N,t}, p_1(t) p_2(t) [V_1^{\varphi_t}, q_1(t)] q_1(t) p_2(t) \psi_{N,t} \rangle \\
&= -\frac{i}{2N} \langle \psi_{N,t}, p_1(t) p_2(t) V_1^{\varphi_t} q_1(t) p_2(t) \psi_{N,t} \rangle.
\end{aligned} \tag{6.40}$$

Here we used (6.38) as well as $p_1(t)q_1(t) = 0$ in the first step and (6.24) in the fourth step to replace $\hat{m}(t)$. Now we can bound (I) trivially by

$$|(I)| \leq \frac{1}{2N} \|V^{\varphi_t}\|_{\infty} = \frac{1}{2N} \|V * |\varphi_t|^2\|_{\infty}. \tag{6.41}$$

Note that now it is the regularity of the Hartree wave function that allows us to control the singularities of V in the right-hand side of (6.41): Indeed, from assumption (A3) we know that

$$V = V^{(1)} + V^{(2)}, \quad V^{(i)} \in L^{p_i}. \tag{6.42}$$

Using Young's inequality, we obtain

$$\|V * |\varphi_t|^2\|_{\infty} \leq \|V^{(1)}\|_{p_1} \|\varphi_t\|_{r_1}^2 + \|V^{(2)}\|_{p_2} \|\varphi_t\|_{r_2}^2, \tag{6.43}$$

where r_1 and r_2 are defined by

$$1 = \frac{1}{p_i} + \frac{2}{r_i}. \tag{6.44}$$

Thus,

$$\|V * |\varphi_t|^2\|_{\infty} \leq (\|V^{(1)}\|_{p_1} + \|V^{(2)}\|_{p_2}) (\|\varphi_t\|_{r_1} + \|\varphi_t\|_{r_2})^2. \tag{6.45}$$

Taking the infimum over all decompositions (6.42) we obtain

$$\|V * |\varphi_t|^2\|_{\infty} \leq \|V\|_{L^{p_1} + L^{p_2}} (\|\varphi_t\|_{r_1} + \|\varphi_t\|_{r_2})^2. \tag{6.46}$$

Observe that the assumptions (A3) and (A4) imply

$$2 \leq r_i \leq q_i \quad \text{for } i = 1, 2. \tag{6.47}$$

Assumption (A4) and L^p -interpolation (8.9) therefore ensure that the right-hand side of (6.46) is finite. Thus

$$|(I)| \leq \frac{1}{2N} \|V\|_{L^{p_1} + L^{p_2}} (\|\varphi_t\|_{r_1} + \|\varphi_t\|_{r_2})^2. \tag{6.48}$$

Estimate of (II): Proceeding analogously as before, we have

$$\begin{aligned}
(II) &= \frac{i}{2} \langle \psi_{N,t}, q_1(t) p_2(t) [(N-1)V_{12} - NV_1^{\varphi_t} - NV_2^{\varphi_t}, \hat{m}(t)] q_1(t) q_2(t) \psi_{N,t} \rangle \\
&= \frac{i}{2} \langle \psi_{N,t}, q_1(t) p_2(t) [\frac{N-1}{N} V_{12} - V_2^{\varphi_t}, q_1(t) + q_2(t)] q_1(t) q_2(t) \psi_{N,t} \rangle \\
&= \frac{i}{2} \langle \psi_{N,t}, q_1(t) p_2(t) \frac{N-1}{N} V_{12} q_1(t) q_2(t) \psi_{N,t} \rangle - \frac{i}{2} \langle \psi_{N,t}, q_1(t) p_2(t) V_2^{\varphi_t} q_1(t) q_2(t) \psi_{N,t} \rangle.
\end{aligned} \tag{6.49}$$

Hence,

$$|(II)| \leq \frac{1}{2} |\langle \psi_{N,t}, q_1(t) p_2(t) V_{12} q_1(t) q_2(t) \psi_{N,t} \rangle| + \frac{1}{2} |\langle \psi_{N,t}, q_1(t) p_2(t) V_2^{\varphi_t} q_1(t) q_2(t) \psi_{N,t} \rangle|. \quad (6.50)$$

By (6.46) the second term of (6.50) is bounded by

$$\begin{aligned} \frac{1}{2} |\langle \psi_{N,t}, q_1(t) p_2(t) V_2^{\varphi_t} q_1(t) q_2(t) \psi_{N,t} \rangle| &= \frac{1}{2} |\langle q_1(t) \psi_{N,t}, p_2(t) V_2^{\varphi_t} q_2(t) q_1(t) \psi_{N,t} \rangle| \\ &\leq \frac{1}{2} \|V^{\varphi_t}\|_{\infty} \|q_1(t) \psi_{N,t}\|_2^2 \\ &\leq \frac{1}{2} \|V\|_{L^{p_1+L^{p_2}}} (\|\varphi_t\|_{r_1} + \|\varphi_t\|_{r_2})^2 \alpha_N(t), \end{aligned} \quad (6.51)$$

where we used that $\|q_1(t) \psi_{N,t}\|_2^2 = \langle \psi_{N,t}, q_1(t) \psi_{N,t} \rangle = \alpha_N(t)$.

Next we bound the first term of (6.50). Using the Cauchy-Schwarz inequality and applying (6.38) to V^2 , we get

$$\begin{aligned} &\frac{1}{2} |\langle \psi_{N,t}, q_1(t) p_2(t) V_{12} q_1(t) q_2(t) \psi_{N,t} \rangle| \\ &\leq \frac{1}{2} \sqrt{\langle \psi_{N,t}, q_1(t) p_2(t) V_{12}^2 p_2(t) q_1(t) \psi_{N,t} \rangle} \sqrt{\langle \psi_{N,t}, q_1(t) q_2(t) \psi_{N,t} \rangle} \\ &= \frac{1}{2} \sqrt{\langle \psi_{N,t}, q_1(t) p_2(t) (V^2 * |\varphi_t|^2)_1 p_2(t) q_1(t) \psi_{N,t} \rangle} \sqrt{\langle \psi_{N,t}, q_1(t) q_2(t) \psi_{N,t} \rangle}. \\ &\leq \frac{1}{2} \sqrt{\|V^2 * |\varphi_t|^2\|_{\infty} \|q_1(t) \psi_{N,t}\|_2^2} \|q_1(t) \psi_{N,t}\|_2 \\ &= \frac{1}{2} \sqrt{\|V^2 * |\varphi_t|^2\|_{\infty}} \alpha_N(t). \end{aligned} \quad (6.52)$$

In order to estimate $\|V^2 * |\varphi_t|^2\|_{\infty}$ we proceed as before. Using the splitting (6.42) and applying Young's inequality we obtain

$$\begin{aligned} \|V^2 * |\varphi_t|^2\|_{\infty} &\leq 2\|(V^{(1)})^2 * |\varphi_t|^2\|_{\infty} + 2\|(V^{(2)})^2 * |\varphi_t|^2\|_{\infty} \\ &\leq 2\|V^{(1)}\|_{p_1}^2 \|\varphi_t\|_{q_1}^2 + 2\|V^{(2)}\|_{p_2}^2 \|\varphi_t\|_{q_2}^2 \\ &\leq 2(\|V^{(1)}\|_{p_1} + \|V^{(2)}\|_{p_2})^2 (\|\varphi_t\|_{q_1} + \|\varphi_t\|_{q_2})^2. \end{aligned} \quad (6.53)$$

Taking the infimum over all decompositions gives

$$\|V^2 * |\varphi_t|^2\|_{\infty} \leq 2\|V\|_{L^{p_1+L^{p_2}}}^2 (\|\varphi_t\|_{q_1} + \|\varphi_t\|_{q_2})^2. \quad (6.54)$$

Hence from (6.51) and (6.52) we finally obtain

$$|(II)| \leq \frac{1}{2} \|V\|_{L^{p_1+L^{p_2}}} \left(\sqrt{2} (\|\varphi_t\|_{q_1} + \|\varphi_t\|_{q_2}) + (\|\varphi_t\|_{r_1} + \|\varphi_t\|_{r_2}) \right) \alpha_N(t). \quad (6.55)$$

Estimate of (III):

$$\begin{aligned}
(III) &= \frac{i}{2} \langle \psi_{N,t}, p_1(t)p_2(t)[(N-1)V_{12} - NV_1^{\varphi_t} - NV_2^{\varphi_t}, \hat{m}(t)]q_1(t)q_2(t)\psi_{N,t} \rangle \\
&= \frac{i}{2} \frac{N-1}{N} \langle \psi_{N,t}, p_1(t)p_2(t)[V_{12}, q_1(t) + q_2(t)]q_1(t)q_2(t)\psi_{N,t} \rangle \\
&= i \frac{N-1}{N} \langle \psi_{N,t}, p_1(t)p_2(t)V_{12}q_1(t)q_2(t)\psi_{N,t} \rangle.
\end{aligned} \tag{6.56}$$

Next, observe that the operator $\hat{n}^{-1}(t) := \sum_{j=0}^N \binom{k}{N}^{-1/2} P_k(t)$ is bounded on the range of $q_1(t)$, because

$$\hat{n}(t)\hat{n}^{-1}(t) = \mathbf{1} - P_0(t) \quad \text{and} \quad P_0(t)q_1(t) = 0. \tag{6.57}$$

Hence,

$$\begin{aligned}
|(III)| &\leq |\langle \psi_{N,t}, p_1(t)p_2(t)V_{12}\hat{n}(t)\hat{n}^{-1}(t)q_1(t)q_2(t)\psi_{N,t} \rangle| \\
&= |\langle \psi_{N,t}, p_1(t)p_2(t)\widehat{\tau_2\hat{n}}(t)V_{12}\hat{n}^{-1}(t)q_1(t)q_2(t)\psi_{N,t} \rangle| \\
&\leq \sqrt{\langle \psi_{N,t}, p_1(t)p_2(t)\widehat{\tau_2\hat{n}}(t)V_{12}^2\widehat{\tau_2\hat{n}}(t)p_1(t)p_2(t)\psi_{N,t} \rangle} \sqrt{\langle \psi_{N,t}, \hat{n}^{-2}(t)q_1(t)q_2(t)\psi_{N,t} \rangle} \\
&\leq \sqrt{\langle \psi_{N,t}, p_1(t)p_2(t)\widehat{\tau_2\hat{n}}(t)(V^2 * |\varphi_t|^2)_1\widehat{\tau_2\hat{n}}(t)p_1(t)p_2(t)\psi_{N,t} \rangle} \sqrt{\frac{N-1}{N}} \sqrt{\alpha_N(t)} \\
&\leq \sqrt{\|V^2 * |\varphi_t|^2\|_\infty} \|\widehat{\tau_2\hat{n}}(t)\psi_{N,t}\|_2 \sqrt{\alpha_N(t)} \\
&\leq \sqrt{\|V^2 * |\varphi_t|^2\|_\infty} \sqrt{\langle \psi_{N,t}, \hat{m}(t)\psi_{N,t} \rangle} + \frac{2}{N} \sqrt{\alpha_N(t)} \\
&= \sqrt{\|V^2 * |\varphi_t|^2\|_\infty} \sqrt{\alpha_N(t)} + \frac{2}{N} \sqrt{\alpha_N(t)} \\
&\leq \sqrt{\|V^2 * |\varphi_t|^2\|_\infty} 2(\alpha_N(t) + \frac{1}{N}).
\end{aligned} \tag{6.58}$$

Here we used Lemma 6.5 in the first step and the Cauchy-Schwarz inequality in the second step. In the third step we applied (6.38) to V^2 and used the fact that

$$\begin{aligned}
\langle \psi_{N,t}, \hat{n}^{-2}(t)q_1(t)q_2(t)\psi_{N,t} \rangle &= \frac{1}{(N-1)N} \sum_{i \neq j}^N \langle \psi_{N,t}, \hat{m}^{-1}(t)q_i(t)q_j(t)\psi_{N,t} \rangle \\
&\leq \frac{1}{(N-1)N} \sum_{i,j=1}^N \langle \psi_{N,t}, \hat{m}^{-1}(t)q_i(t)q_j(t)\psi_{N,t} \rangle \\
&= \frac{N}{N-1} \langle \psi_{N,t}, \hat{m}^{-1}(t)\hat{m}^2(t)\psi_{N,t} \rangle \\
&= \frac{N}{N-1} \alpha_N(t).
\end{aligned} \tag{6.59}$$

Moreover, in the fourth step we used

$$\|\widehat{\tau_2\hat{n}}(t)\psi_{N,t}\|_2 = \sqrt{\langle \psi_{N,t}, \widehat{\tau_2\hat{m}}(t)\psi_{N,t} \rangle} \leq \sqrt{\langle \psi_{N,t}, \hat{m}(t)\psi_{N,t} \rangle} + \frac{2}{N}. \tag{6.60}$$

Inserting the estimates (6.48), (6.55) and (6.58) into (6.37) yields

$$|\dot{\alpha}_N(t)| \leq 4|(I)| + 4|(II)| + 2|(III)| \leq \frac{1}{N}B_N(t) + B_N(t)\alpha_N(t), \quad (6.61)$$

where

$$B_N(t) := 2\|V\|_{L^{p_1+L^{p_2}}} (6(\|\varphi_t\|_{q_1} + \|\varphi_t\|_{q_2}) + (\|\varphi_t\|_{r_1} + \|\varphi_t\|_{r_2})^2). \quad (6.62)$$

Using L^2 -norm conservation $\|\varphi_t\|_2 = 1$ and $2 \leq r_i \leq q_i$, we obtain by L^p -interpolation (8.9) that $\|\varphi_t\|_{r_i}^2 \leq \|\varphi_t\|_{q_i}$. Hence,

$$B_N(t) \leq 16\|V\|_{L^{p_1+L^{p_2}}} (\|\varphi_t\|_{q_1} + \|\varphi_t\|_{q_2}). \quad (6.63)$$

Finally, coming back to the Grönwall estimate,

$$\alpha_N(t) \leq (\alpha_N(0) + \frac{1}{N}) \left(\int_0^t ds B_N(s) \right) e^{\int_0^t ds B_N(s)} \leq (\alpha_N(0) + \frac{1}{N}) e^{2 \int_0^t ds B_N(s)}, \quad (6.64)$$

which completes the proof. \square

6.2 Inclusion of a magnetic field

We can now state the strongest result of this thesis. We prove that with the projections method one can include a reasonably general class of external magnetic fields. The overall result for three dimensions is as follows.

Theorem 6.6. *Let $V \in L^\infty(\mathbb{R}^3)$ or $V(x) = \frac{\lambda}{|x|}$, $\lambda \in \mathbb{R}$, and assume that the magnetic vector potential $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ satisfies assumption (A). We consider the mean-field quantum dynamics generated by the Hamiltonian*

$$H_N = \sum_{j=1}^N (-i\nabla_{x_j} + A(x_j))^2 + \frac{1}{N} \sum_{i<j}^N V(x_i - x_j). \quad (6.65)$$

Let $\varphi \in H_A^1(\mathbb{R}^3)$ with $\|\varphi\|_2 = 1$ and set $\psi_N = \varphi^{\otimes N}$. Let $\psi_{N,t} = e^{-iH_N t} \psi_N$ and denote by φ_t the solution to the magnetic Hartree equation (3.3) with initial data $\varphi_{t=0} = \varphi$. Denote by $\gamma_{N,t}^{(k)}$ the k -particle marginals associated with $\psi_{N,t}$. Then there exists a constant $C > 0$ such that, for $k \in \mathbb{N}$ and $t \in \mathbb{R}$,

$$\mathrm{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right| \leq 2 \sqrt{\frac{k}{N}} e^{Ct} \quad (6.66)$$

holds for all $N \geq k$. In particular, this implies for every fixed $k \in \mathbb{N}$ and every fixed $t \in \mathbb{R}$

$$\lim_{N \rightarrow \infty} \mathrm{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right| = 0. \quad (6.67)$$

Proof. Assume that $V(x) = \frac{\lambda}{|x|}$, $\lambda \in \mathbb{R}$. The case $V \in L^\infty(\mathbb{R}^3)$ is easier and therefore omitted. We will verify the assumptions (A1), (A2), (A3') and (A4'). The assertion then follows from Theorem 6.1, Corollary 6.2 and Remark 6.4.

Note that the form domain X_1 is the magnetic Sobolev space $H_A^1(\mathbb{R}^3)$.

(A1) The one-particle Hamiltonian $h = (-i\nabla + A)^2$ is positive and self-adjoint by Theorem 2 in Leinfelder and Simader [26].

(A2) Theorem X.16 and Example 2 in Section X.2 in [31] show that the operator $H_N^V = \sum_{i < j}^N \frac{\lambda}{|x_i - x_j|}$ is infinitesimally small with respect to the operator $\sum_{j=1}^N -\Delta_j$. Theorem 2.4 in [1] then implies that H_N^V is also infinitesimally small with respect to $H_N^0 = \sum_{j=1}^N (-i\nabla_j + A)^2$. Hence, by the Kato-Rellich Theorem 8.12, H_N is self-adjoint on the domain $D(H_N^0)$ of H_N^0 and bounded from below.

Moreover, this implies that H_N^0 is H_N -bounded. Using Theorem X.18 in [31], we infer that H_N^0 is form-bounded with respect to H_N . By the definition of form-boundedness, $\mathcal{Q}(H_N) \subset \mathcal{Q}(H_N^0)$.

(A3') The Coulomb interaction potential $V(x) = \frac{\lambda}{|x|}$, $\lambda \in \mathbb{R}$, is a real and even function. For every $\varphi \in H_A^1(\mathbb{R}^3)$ we have

$$\begin{aligned} \|V^2 * |\varphi|^2\|_\infty &= \sup_{x \in \mathbb{R}^3} \left| \int_{\mathbb{R}^3} \frac{\lambda^2}{|x-y|^2} |\varphi(y)|^2 dy \right| \\ &\leq 4\lambda^2 \|\nabla_{x-y} |\varphi|\|_2^2 \\ &= 4\lambda^2 \|\nabla_x |\varphi|\|_2^2 \\ &\leq 4\lambda^2 \|(-i\nabla_x + A)\varphi\|_2^2 \\ &\leq 4\lambda^2 \|\varphi\|_{H_A^1}^2. \end{aligned} \tag{6.68}$$

Here we used Hardy's inequality (8.10) in the second line, the translational invariance of ∇ in the third line and the diamagnetic inequality (8.11) in the fourth line.

(A4') Theorem 3.3 states that the solution φ_t of the magnetic Hartree equation (3.3) with initial data φ satisfies

$$\varphi_t \in C(\mathbb{R}; H_A^1) \cap C^1(\mathbb{R}; H_A^{-1}) \tag{6.69}$$

and that furthermore, we have $\sup \{\|\varphi_t\|_{H_A^1} \mid t \in \mathbb{R}\} < \infty$. Thus

$$\phi(t) = 32K \int_0^t ds \|\varphi_s\|_{H_A^1}^2 \leq 32K \left(\sup \{\|\varphi_t\|_{H_A^1} \mid t \in \mathbb{R}\} \right)^2 t. \tag{6.70}$$

Hence, for every $k \in \mathbb{N}$ and $t \in \mathbb{R}$, we have

$$\mathrm{tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle \langle \varphi_t|^{\otimes k} \right| \leq 2\sqrt{\frac{k}{N}} e^{\phi(t)/2} \leq 2\sqrt{\frac{k}{N}} e^{Ct} \tag{6.71}$$

with $C \equiv 16K \left(\sup \{\|\varphi_t\|_{H_A^1} \mid t \in \mathbb{R}\} \right)^2$, which completes the proof. \square

Remark 6.7. Note that the verification of the global well-posedness of the magnetic Hartree equation (3.3) in (A4') required the biggest effort in the proof of Theorem 6.6. This was worked out in Chapter 3.

Remark 6.8. Theorem 6.6 also holds for the class of potentials $V \in L^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. For example, all potentials of the type $V(x) = \frac{\lambda}{|x|^\alpha}$, $\lambda \in \mathbb{R}$ and $0 \leq \alpha < 1$, belong to this class. We now sketch briefly how to verify (A2), (A3') and (A4') for this class of potentials.

(A2) If $V \in L^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, then also $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Since all potentials $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ are $-\Delta$ -bounded (see e.g. the proof of Theorem X.15 in [31]), the same argument as above applies.

(A3') Let $V \equiv V_1 + V_2 \in L^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with $V_1 \in L^3(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$, and let $\varphi \in H_A^1(\mathbb{R}^3)$. Then

$$\begin{aligned}
\|V^2 * |\varphi|^2\|_\infty &= \sup_{x \in \mathbb{R}^3} \left| \int_{\mathbb{R}^3} |V(x-y)|^2 |\varphi(y)|^2 dy \right| \\
&\leq 2 \sup_{x \in \mathbb{R}^3} \left| \int_{\mathbb{R}^3} (|V_1(x-y)|^2 + |V_2(x-y)|^2) |\varphi(y)|^2 dy \right| \\
&\leq 2 \sup_{x \in \mathbb{R}^3} \left| \int_{\mathbb{R}^3} |V_1(x-y)|^2 |\varphi(y)|^2 dy \right| + 2 \|V_2\|_\infty \|\varphi\|_2^2 \\
&\leq 2 \|V_1\|_3^2 \|\varphi\|_6^2 + 2 \|V_2\|_\infty \|\varphi\|_2^2 \\
&\leq 2C \|V_1\|_3^2 \|\nabla|\varphi|\|_2^2 + 2 \|V_2\|_\infty \|\varphi\|_2^2 \\
&\leq 2C \|V_1\|_3^2 \|(-i\nabla + A)\varphi\|_2^2 + 2 \|V_2\|_\infty \|\varphi\|_2^2 \\
&\leq (2C \|V_1\|_3^2 + 2 \|V_2\|_\infty) \|\varphi\|_{H_A^1}^2.
\end{aligned} \tag{6.72}$$

Here we used the Hölder inequality in the fourth line, the Sobolev inequality in the fifth line and the diamagnetic inequality (8.11) in the sixth line.

(A4') This follows from Theorem 3.4 and Remark 3.12 (notice that $V \in L^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ implies $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$).

Chapter 7

Conclusion

In this thesis three different approaches to the study of mean-field quantum dynamics have been reviewed. It proved possible to adapt these methods to include a magnetic field in three dimensions. This required several non-trivial modifications of the methods. In particular, it was necessary to establish the global well-posedness of the magnetic Hartree equation (3.3). The results pertain to a reasonable class of magnetic vector potentials satisfying the assumption **(A)**. This includes the physically relevant case of a constant magnetic field.

For bounded interaction potentials V , a magnetic field could be included by all three methods. The perturbative expansion of the BBGKY hierarchy in Chapter 4 and the compactness argument in Chapter 5 both gave the convergence (1.18) to the limiting dynamics determined by the solution to the magnetic Hartree equation. The compactness argument is considerably more involved than the perturbative expansion and does not yield a better result. However, among the two methods, only the compactness method might be extendable to the case of including a magnetic field for singular interaction potentials. This would be an interesting topic to pursue further.

The projections method was used in Chapter 6 to include a magnetic field not only for bounded potentials, but also for the Coulomb potential. Moreover, an estimate on the rate of convergence of (1.18) was attained. This approach therefore gave the strongest result obtained in this work.

It is desirable to extend these results to a larger class of magnetic vector potentials. The methods in Chapters 4, 5 and 6 would allow this. However, the necessary global well-posedness of the magnetic Hartree equation depends crucially on the class of vector potentials satisfying the assumption **(A)**. For those vector potentials the magnetic Strichartz's estimates by Yajima hold. These estimates are at the heart of the proof of global well-posedness in Chapter 3. Suitable magnetic Strichartz's estimates, allowing e.g. for less regular vector potentials without decay assumptions, would immediately improve our results.

Furthermore, it would be interesting to find out whether one can also include a magnetic field in arbitrary dimension $d \geq 2$. The magnetic Strichartz's estimates by Yajima hold for all dimensions $d \geq 2$. For bounded interaction potentials V , the global well-posedness of the magnetic Hartree equation can then be derived in exactly the same way as in Chapter 3.

For bounded potentials, the approaches in Chapters 4 and 6 apply without change for any dimension $d \geq 2$. For the compactness argument in Chapter 5 to work, minor modifications have to be made. The proof of Proposition 5.6 relies on showing the compactness of the operator (5.39). The presented proof of the latter does not go through in higher dimensions, one would have to introduce additional cut-offs. However, Proposition 5.10 is the crucial ingredient of the second approach to the proof of Proposition 5.6. Its proof can be easily generalised to arbitrary dimensions. It suffices to go through the same scheme of (5.64) using the general form (8.14) of the relativistic heat kernel.

For the potential $V(x) = \frac{\lambda}{|x|}$, $\lambda \in \mathbb{R}$, in dimensions $d \geq 3$, the global well-posedness of the magnetic Hartree equation can actually be established. Moreover, the projections method in Chapter 6 to include a magnetic field in the mean-field quantum dynamics also works for this potential. Both cases rely essentially on applying Hardy's inequality (8.10) and the diamagnetic inequality (8.11). These inequalities hold for all $d \geq 3$.

Chapter 8

Appendix

8.1 Partial trace and reduced density matrices

In the following let $\mathcal{H}_1, \mathcal{H}_2$ be two separable Hilbert spaces and set $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$.

Definition 8.1. Let T be a trace class operator on the tensor product \mathcal{H} . There then exists a unique operator $\text{tr}_{\mathcal{H}_2} T \in \mathcal{L}^1(\mathcal{H}_1)$ such that

$$\text{tr}(\text{tr}_{\mathcal{H}_2} T)A = \text{tr} T(A \otimes \mathbb{1}_{\mathcal{H}_2}) \quad (8.1)$$

holds for every compact operator $A \in \mathcal{K}(\mathcal{H}_1)$. This operator $\text{tr}_{\mathcal{H}_2} T$ is called the partial trace of T with respect to \mathcal{H}_2 . Note that on the left-hand side of (8.1), the trace is taken on $\mathcal{L}^1(\mathcal{H}_1)$, while on the right-hand side it is taken on $\mathcal{L}^1(\mathcal{H})$.

The existence of the partial trace follows from duality: The mapping $A \mapsto \text{tr} T(A \otimes \mathbb{1}_{\mathcal{H}_2})$ is a bounded linear functional on $\mathcal{K}(\mathcal{H}_1)$ and $\mathcal{K}(\mathcal{H}_1)^* = \mathcal{L}^1(\mathcal{H}_1)$. One can show that the partial trace $\text{tr}_{\mathcal{H}_2} T \in \mathcal{L}^1(\mathcal{H}_1)$ is equivalently characterised by requiring that, for any orthonormal basis $\{\xi_j\}_{j \in \mathbb{N}}$ of \mathcal{H}_2 , we have

$$\langle \varphi, (\text{tr}_{\mathcal{H}_2} T)\psi \rangle_{\mathcal{H}_1} = \sum_{j=1}^{\infty} \langle \varphi \otimes \xi_j, T\psi \otimes \xi_j \rangle_{\mathcal{H}} \quad \forall \varphi, \psi \in \mathcal{H}_1. \quad (8.2)$$

Proposition 8.2. The partial trace satisfies the following relations:

$$\text{tr} \text{tr}_{\mathcal{H}_2}(T) = \text{tr} T \quad \forall T \in \mathcal{L}^1(\mathcal{H}) \quad (8.3)$$

$$T \geq 0 \Rightarrow \text{tr}_{\mathcal{H}_2}(T) \geq 0 \quad \forall T \in \mathcal{L}^1(\mathcal{H}) \quad (8.4)$$

$$\text{tr}_{\mathcal{H}_2}(T_1 \otimes T_2) = T_1 \cdot \text{tr} T_2 \quad \forall T_1 \in \mathcal{L}^1(\mathcal{H}_1) \quad \forall T_2 \in \mathcal{L}^1(\mathcal{H}_2) \quad (8.5)$$

$$\text{tr} |\text{tr}_{\mathcal{H}_2}(T)| \leq \text{tr} |T| \quad \forall T \in \mathcal{L}^1(\mathcal{H}). \quad (8.6)$$

Definition 8.3. A density matrix on a Hilbert space is a positive self-adjoint trace class operator with unit trace.

Suppose γ is a density matrix on $\mathcal{H}_1 \otimes \mathcal{H}_2$. Then by (8.3) and (8.4), the partial trace $\text{tr}_{\mathcal{H}_2}(\gamma)$ is a density matrix on \mathcal{H}_1 . It is called the *reduced density matrix* of γ with respect to \mathcal{H}_1 .

If the Hilbert space is $L^2(\mathbb{R}^n)$, the operation of taking the partial trace on density matrices can be formulated in terms of kernels.

Proposition 8.4. *Let $\mathcal{H}_1 = L^2(\mathbb{R}^n)$ and $\mathcal{H}_2 = L^2(\mathbb{R}^m)$ for some $n, m \in \mathbb{N}$ and let γ be a density matrix on $\mathcal{H}_1 \otimes \mathcal{H}_2$ with integral kernel $\gamma(x, y; x', y')$. Then $\text{tr}_{\mathcal{H}_2}(\gamma)$ has integral kernel*

$$\gamma^{(\mathcal{H}_2)}(x; x') = \int_{\mathbb{R}^m} dy \gamma(x, y; x', y), \quad (8.7)$$

where the integral is rigorously defined via the canonical decomposition of γ in terms of its eigenfunctions.

See the appendix in [12] or Chapter 2 in [30] for more information on partial trace and density matrices.

8.2 L^p - estimates

Theorem 8.5 (Young's inequality). *Let $1 \leq p, q, r \leq \infty$ with $1 + \frac{1}{r} = \frac{1}{p} + \frac{1}{q}$ and let $f \in L^p(\mathbb{R}^d)$, $g \in L^q(\mathbb{R}^d)$. Then*

$$\|f * g\|_r \leq \|f\|_p \|g\|_q. \quad (8.8)$$

Theorem 8.6 (L^p -interpolation). *Let $1 \leq p \leq q \leq \infty$ and let $f \in L^p(\mathbb{R}^d) \cap L^q(\mathbb{R}^d)$. Let $\theta \in (0, 1)$ and define r by $\frac{1}{r} = \frac{\theta}{p} + \frac{1-\theta}{q}$. Then $f \in L^r(\mathbb{R}^d)$ and*

$$\|f\|_r \leq \|f\|_p^\theta \|f\|_q^{1-\theta}. \quad (8.9)$$

Theorem 8.7 (Hardy's inequality). *For any $d \geq 3$ and $\psi \in H^1(\mathbb{R}^d)$ we have*

$$\frac{(d-2)^2}{4} \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2} dx \leq \int_{\mathbb{R}^d} |\nabla \psi(x)|^2 dx. \quad (8.10)$$

8.3 Diamagnetic inequalities

Proposition 8.8 (Diamagnetic inequality). *Let $A \in L^2_{loc}(\mathbb{R}^d; \mathbb{R}^d)$ and let $\varphi \in H^1_A(\mathbb{R}^d)$. Then $|\varphi| \in H^1(\mathbb{R}^d)$ and the diamagnetic inequality*

$$|\nabla |\varphi|(x)| \leq |(-i\nabla + A)\varphi(x)| \quad (8.11)$$

holds pointwise for almost every $x \in \mathbb{R}^d$.

Proof. See Theorem 7.21 in [27]. □

Theorem 8.9 (Non-relativistic diamagnetic inequality). *Let $A \in L^2_{loc}(\mathbb{R}^d; \mathbb{R}^d)$. Then, for $e > 0$ and for almost every $x, y \in \mathbb{R}^d$,*

$$\left| \frac{1}{e + (-i\nabla + A(x))^2}(x, y) \right| \leq \frac{1}{e - \Delta}(x, y). \quad (8.12)$$

Proof. See Theorem 4.4 in [28]. □

Theorem 8.10 (Relativistic diamagnetic inequality). *Let $A \in L^2_{loc}(\mathbb{R}^d; \mathbb{R}^d)$. Then, for $e > 0$ and for almost every $x, y \in \mathbb{R}^d$,*

$$\left| \frac{1}{e + |-i\nabla + A(x)|}(x, y) \right| \leq \frac{1}{e + \sqrt{-\Delta}}(x, y). \quad (8.13)$$

The relativistic heat kernel at $t > 0$ is given by

$$e^{-t\sqrt{-\Delta}}(x, y) = \Gamma\left(\frac{d+1}{4}\right)\pi^{-(d+1)/2} \frac{t}{(t^2 + |x - y|^2)^{(d+1)/2}}. \quad (8.14)$$

Proof. See Theorem 4.4 in [28]. □

8.4 Kato-Rellich - Theorem

Definition 8.11. *Let A and B be densely defined linear operators on a Hilbert space \mathcal{H} with norm $\|\cdot\|$. Suppose that:*

- (i) $D(B) \supset D(A)$
- (ii) For some $a, b \in \mathbb{R}$ and all $\varphi \in D(A)$,

$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\|. \quad (8.15)$$

Then B is said to be A -bounded. The infimum of such a is called the relative bound of B with respect to A . If the relative bound is zero, we say that B is infinitesimally small with respect to A .

Theorem 8.12 (Kato-Rellich). *Suppose that A is self-adjoint, B is symmetric, and B is A -bounded with relative bound $a < 1$. Then $A + B$ is self-adjoint on $D(A)$ and essentially self-adjoint on any core of A . Further, if A is bounded from below by M , then $A + B$ is bounded from below by $M - \max\{b/(1 - a), a|M| + b\}$, where a and b are given by (8.15).*

Proof. See Theorem X.12 in [31]. □

8.5 $f(x)g(-i\nabla)$ - Theorem

Theorem 8.13. *Let $f, g \in L^2(\mathbb{R}^d)$ and define an operator $f(\cdot)g(-i\nabla) : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ by*

$$(f(\cdot)g(-i\nabla)\psi)(x) = f(x)(g(\cdot)\hat{\psi})^\vee(x), \quad \psi \in L^2(\mathbb{R}^d). \quad (8.16)$$

Then

$$\|f(x)g(-i\nabla)\|_{\mathcal{L}^2} = \frac{1}{(2\pi)^{d/2}} \|f\|_2 \|g\|_2. \quad (8.17)$$

In particular, if f and g are in the L^∞ - closure of $L^2(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$, then the operator $f(\cdot)g(-i\nabla)$ is compact.

Proof. See the proof of Theorem 4.1 in [36]. □

8.6 Grönwall - Lemma

Lemma 8.14 (Grönwall). *Let $\eta(\cdot)$ be a nonnegative, absolutely continuous function on $[0, T]$, which satisfies for a.e. t the differential inequality*

$$\eta'(t) \leq \psi(t) + \phi(t)\eta(t), \quad (8.18)$$

where $\psi(t)$ and $\phi(t)$ are nonnegative, summable functions on $[0, T]$. Then

$$\eta(t) \leq \left(\eta(0) + \int_0^t ds \psi(s) \right) e^{\int_0^t ds \phi(s)} \quad (8.19)$$

for all $0 \leq t \leq T$.

Proof. See e.g. Section (j) of the Appendix B in [15]. □

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