Conservative Quantum Dynamical Semigroups for a Class of Mean Field Master Equations

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Abstract

We consider a class of evolution equations in Lindblad form, which model the dynamics of dissipative quantum mechanical systems with mean field interaction. Particularly, this class includes the so-called Quantum Fokker-Planck-Poisson model. The existence and uniqueness of global, mass preserving solutions is proved, thus establishing the existence of a nonlinear conservative quantum dynamical semigroup.

Key words: open quantum system, Lindblad operators, quantum dynamical semigroup, dissipative operators, density matrix

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1 Introduction

We consider a quantum mechanical system coupled to its surrounding, *i.e.* a so called *open quantum system* [Da], [BrPe]. In this case, the Hamiltonian dynamics, appropriate for an isolated system, needs to be replaced by a more general class of dynamical maps. In the *Schrödinger picture*, such a map Φ_t acts on the space of density matrices ρ, or, more precisely, on the space of positive self-adjoint trace class operators $\rho \in \mathcal{J}_1(\mathcal{H})$ over some *Hilbert space* $\mathcal{H}$, say $L^2(\mathbb{R}^d)$.

In the *Markovian regime*, *i.e.* if no memory effects appear in the dynamics, Φ_t satisfies the semigroup property. A semigroup Φ_t which is strongly continuous, completely positive and which additionally preserves the trace on $\mathcal{J}_1$, *i.e.* the *mass* of the particles, is called a *conservative quantum dynamical semigroup*

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(QDS). We refer to [FaRe] for a modern (mathematical) introduction to the theory of QDS and to [Al], [AlFa], [BrPe], [Sp] for physical applications.

Any QDS can be represented by $\Phi_t(\rho_0) = e^{\mathcal{L}t}\rho_0$. Its generator $\mathcal{L}$, governs the time-evolution of $\rho(t)$, through a so-called *Markovian master equation*,

$$\begin{cases} \dfrac{d}{dt}\rho = \mathcal{L}(\rho), \quad t > 0, \\ \rho\big|_{t=0} = \rho_0 \in \mathcal{J}_1. \end{cases}$$

It is well known that, if $\mathcal{L}$ is a bounded operator, it has to be in the so called *Lindblad class* [Li] in order to define a completely positive (and conservative) QDS (the same result has been proved independently in [GKS]). In most cases, however, $\mathcal{L}$ is unbounded and so far no complete characterization of admissible generators, in the above sense, is known.

Indeed, already more than 20 years ago, E. B. Davies showed in his classical work [Da1], that it is possible to construct, for a quite general class of unbounded Lindblad generators $\mathcal{L}$, a so called *minimal solution* to the above master equation. However, this construction in general is not unique, *i.e.* the formal (unbounded) generator $\mathcal{L}$ does not uniquely determine a corresponding QDS. This in particular implies that the minimal solution may not be trace preserving, *cf.* example 3.3 in [Da1]. From a physical point of view it seems that nonconservative (sometimes called *explosive*) solutions are reasonable only in situations where particles can be created or annihilated as discussed for example in [Da], [Da1]. A recent mathematical study of such *nonconservative* minimal solution can be found in [Qu].

Nowadays, various sufficient conditions for conservativity can be found in [ChFa], [CGQ], and in [Ho], where additionally certain covariance properties on the generator $\mathcal{L}$ are imposed. For many concrete examples, however, these conditions are rather difficult to verify, as we shall discuss in more detail at the end of section 3.

The present work establishes the existence and uniqueness of a conservative quantum dynamical semigroup for a concrete family of unbounded operators $\mathcal{L}$, which are formally in the Lindblad class. The considered Lindblad operators, which represent the influence of the environment, are linear combinations of the position and momentum operators. This particular choice of operators is motivated by the physically interesting *Quantum Fokker-Planck models*, which frequently appear in the literature on open quantum systems. (Concrete applications of such equations are discussed at the end of section 2.) So far, only partial results on the rigorous derivation of these models from many-body quantum dynamics are available. In this context, our work (at least) shows that such models indeed generate a conservative QDS, *i.e.* they satisfy the *basic physical requirements.*

Throughout this paper, we shall work in the Schrödinger picture, which is more appropriate in our case. We consider a system coupled to its environment and, moreover, we include the possible interaction of the particles with each other, in our case modelled by a mean field approximation of *Hartee* type (extensions to *Hartee-Fock* systems would be possible by using techniques as in [ABJZ]). More precisely, we consider the master equation to be self-consistently coupled to the *Poisson equation*

$$\Delta\phi = -\kappa n, \quad \kappa = \pm 1,$$

where $n = n[\rho]$ is the particle density computed from ρ. The choice of the coupling constant $\kappa = \pm 1$ corresponds, respectively, to the (usual) repulsive and attracting case (see [Lie] for a quantum-attractive model). In the following, we shall analyze only the repulsive case. However, using modified a-priori energy estimates (as in [Ar]) it is possible to include the case $\kappa = -1$.

We remark that the literature of rigorous studies of QDS has mainly focused on linear master equations (see *e.g.* the works quoted above). To the authors' knowledge the only results including nonlinear effects are [Ar1] and [AlMe], which, however, can not be applied directly to our case.

This paper is organized as follows:

After introducing the model in section 2 we will prove in section 3 existence and uniqueness of global, mass preserving solutions, *i.e.* existence of a conservative QDS, to the linear equation. A crucial analytical tool towards this end is a new density lemma (relating minimal and maximal operator realizations) for Lindblad generators $\mathcal{L}$ that are quadratic in the position and momentum operator. The mean field will then be included in section 4 (we shall restrict ourselves for simplicity to the case of $d = 3$ spatial dimensions). We prove that the self-consistent potential is a locally Lipschitz perturbation of the free evolution in an appropriate "energy space", and this yields a local-in-time existence and uniqueness result. Finally, we shall prove global existence of a conservative QDS in section 5 by establishing a-priori estimates for the mass and total energy of the system.

2 The model equation

Throughout this work we set the physical constants $\hbar = m = e = 1$, for simplicity.

In the sequel we shall use the following standard notations:

Definition 2.1. An operator A is *trace class*, if

$$|||A|||_1 := \operatorname{Tr}|A| < \infty \tag{2.1}$$

and it is *Hilbert-Schmidt*, if

$$|||A|||_2 := \left(\operatorname{Tr}|A|^2\right)^{\frac{1}{2}} < \infty, \tag{2.2}$$

where Tr denotes the usual operator trace on $\mathcal{B}(L^2(\mathbb{R}^d))$ (bounded operators). The corresponding *spaces* of operators are denoted by $\mathcal{J}_1$ and $\mathcal{J}_2$, respectively. If A is trace-class *and self-adjoint*, we shall write $A \in \tilde{\mathcal{J}}_1 \subset \mathcal{J}_1$. Finally, denoting by $\|\cdot\|_p$, $1 \le p \le \infty$, the usual $L^p(\mathbb{R}^d)$-norm, we write

$$|||A|||_\infty := \sup_f \|Af\|_2, \quad f \in \mathcal{D}(A), \ \|f\|_2 = 1, \tag{2.3}$$

for the *operator norm* of $A \in \mathcal{B}(L^2(\mathbb{R}^d))$ with domain of definition $\mathcal{D}(A)$.

We consider open quantum systems of massive, *spin-less* particles within an *effective single-particle approximation*, as it has been studied for example in [CEFM]. Hence, at every time $t \in \mathbb{R}$ a physically relevant, *mixed state* of our system is uniquely given by a positive operator $\rho(t) \in \tilde{\mathcal{J}}_1$, in the sequel called *density matrix operator.* Since ρ is also Hilbert-Schmidt it can be represented by an integral operator $\rho(t) : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$, *i.e.*

$$(\rho(t)f)(x) := \int_{\mathbb{R}^d} \rho(x, y, t) f(y) dy. \tag{2.4}$$

Its kernel $\rho(\cdot, \cdot, t) \in L^2(\mathbb{R}^{2d})$ is then called the *density matrix function* of the state ρ. By abuse of notation we shall identify from now on the operator $\rho \in \tilde{\mathcal{J}}_1$ with its kernel $\rho(\cdot, \cdot) \in L^2(\mathbb{R}^{2d})$. It is well known [ReSi1] that $|||\rho|||_2 = \|\rho\|_2$, *i.e.*

$$\left(\operatorname{Tr} |\rho|^2\right)^{\frac{1}{2}} = \left(\int\int_{\mathbb{R}^d \times \mathbb{R}^d} |\rho(x, y)|^2 dx dy\right)^{\frac{1}{2}}. \tag{2.5}$$

Further, it is known that every density matrix operator ρ possesses a diagonal Fourier expansion of the form

$$\rho(x, y) = \sum_{j \in \mathbb{N}} \lambda_j \ \psi_j(x) \overline{\psi_j(y)}, \tag{2.6}$$

where $\{\lambda_j\} \in l^1(\mathbb{N})$, $\lambda_j \geq 0$, and the complete o.n.s. $\{\psi_j\} \subset L^2(\mathbb{R}^d)$ are the eigenvalues and eigenfunctions of ρ. The λ_j represent the occupation probability of the pure state ψ_j. Note that for self-adjoint $\rho \geq 0$ the trace norm is equal to

$$|||\rho|||_1 := \operatorname{Tr} |\rho| = \operatorname{Tr} \rho = \sum_{j \in \mathbb{N}} \lambda_j. \tag{2.7}$$

Using equation (2.6) one can define the *particle density* $n[\rho]$ by setting $x = y$, to obtain

$$n[\rho](x) := \sum_{j \in \mathbb{N}} \lambda_j \ |\psi_j(x)|^2, \quad x \in \mathbb{R}^d. \tag{2.8}$$

However, since $\{x = y\} \subset \mathbb{R}^{2d}$ is a set of measure zero, this is not a mathematically rigorous procedure for a kernel $\rho(x, y)$ that is merely in $L^2(\mathbb{R}^{2d})$. On the other hand, if $\rho(x, y)$ is indeed the kernel of an operator $\rho \in \mathcal{J}_1$ it is known, *cf.* [Ar], [LiPa], that the particle density can be rigorously defined by

$$n[\rho](x) := \lim_{\varepsilon \to 0} \int_{\mathbb{R}^d} \rho\left(x + \frac{\eta}{2}, x - \frac{\eta}{2}\right) \frac{e^{-|\eta|^2/2\varepsilon}}{(2\pi\varepsilon)^{d/2}} \, d\eta \in L^1_+(\mathbb{R}^d). \tag{2.9}$$

And it satisfies $\|n\|_1 = \operatorname{Tr}(\rho)$ for $\rho \geq 0$. This issue of rigorously defining $n[\rho]$ is one of the mathematical motivations for analyzing our mean field evolution equations as an abstract evolution problem for the operator ρ on the Banach space $\tilde{\mathcal{J}}_1$ (and not as a technically much easier PDE for the function ρ on $L^2(\mathbb{R}^{2d})$).

Remark 2.2. Note that we can not use the decomposition (2.6) in order to pass to a PDE problem for the ψ_j, since the considered dissipative evolution equation in general does not conserve the occupation probabilities λ_j. This is in sharp contrast to unitary dynamical maps generated by the von Neumann equation of standard quantum mechanics.

We consider the following (nonlinear) dissipative equation modeling the motion of particles, interacting with each other and with their environment

$$\begin{cases} \frac{d}{dt}\rho = -i\,[H,\rho] + A(\rho), \quad t > 0, \\ \rho\big|_{t=0} = \rho_0 \in \tilde{\mathcal{J}}_1. \end{cases} \tag{2.10}$$

Here, $[\cdot,\cdot]$ is the commutator bracket, H and $A(\rho)$ are formally self-adjoint and of Lindblad class. More precisely, we consider the *Hamiltonian operator*

$$H := -\frac{\Delta}{2} + V[\rho](x,t) - i\mu[x,\nabla]_+, \quad \mu \in \mathbb{R}, \tag{2.11}$$

denoting by $[\cdot,\cdot]_+$ the anti-commutator. The operators x and ∇ are, respectively, the multiplication and gradient operator on $\mathbb{R}^d$, *i.e.* $[x,\nabla]_+ = x\cdot\nabla + \nabla\cdot x = 2x\cdot\nabla + d$.

Remark 2.3. The operator H is sometimes called *adjusted Hamiltonian*, due to the appearence of the $[x,\nabla]_+$- term. Depending on the particular model, such a term may [ALMS] or may not be present [Va]. Nevertheless it is included here, in order to keep our presentation as general as possible.

The (real-valued) potential V is assumed to be of the form

$$V[\rho](x,t) := \frac{|x|^2}{2} + V_1(x) + \phi[\rho](x,t), \quad x \in \mathbb{R}^d, \tag{2.12}$$

where the first term of the r.h.s. denotes a possible confinement potential and $V_1 \in L^\infty(\mathbb{R}^d)$ is a bounded perturbation of it. ϕ is the *Hartree-* or *mean field-potential*, obtained from the *self-consistent* coupling to the *Poisson equation*

$$\Delta\phi[\rho] = -n[\rho]. \tag{2.13}$$

For $d = 3$, we therefore get the usual Hartree-term:

$$\phi[\rho](x,t) = \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{n[\rho](y,t)}{|x-y|}\, dy, \quad x, y \in \mathbb{R}^3, \tag{2.14}$$

where n is computed from ρ by (2.9). This mean field approximation describes the (repulsive) Coulombian interaction of the particles with each other.
The non-Hamiltonian part is defined as

$$A(\rho) := \sum_{j=1}^{M} L_j\rho L_j^* - \frac{1}{2}\left[L_j^* L_j, \rho\right]_+, \quad M \in \mathbb{N}, \tag{2.15}$$

or equivalently

$$A(\rho) = \sum_{j=1}^{M} \frac{1}{2}\left[L_j\rho, L_j^*\right] + \frac{1}{2}\left[L_j, \rho L_j^*\right], \tag{2.16}$$

where the linear operators L_j (*Lindblad operators*) are assumed to be of the form

$$L_j := \alpha_j\cdot x + \beta_j\cdot\nabla + \gamma_j, \quad \alpha_j, \beta_j \in \mathbb{C}^d, \gamma_j \in \mathbb{C}. \tag{2.17}$$

Its adjoint is $L_j^* = \bar{\alpha}_j \cdot x - \bar{\beta}_j \cdot \nabla + \bar{\gamma}_j$, and in the following we shall use the notation

$$L := \sum_{j=1}^{M} L_j^* L_j. \tag{2.18}$$

Remark 2.4. In the framework of *second quantization* and in $d = 1$, the space $L^2(\mathbb{R})$ is unitarily mapped onto $\mathcal{F}_s(\mathbb{C})$, the *symetric* or *bosonic Fock space* over $\mathbb{C}$. This space is frequently used, for example in quantum optics, in order to describe *two − level* bosonic systems, *cf.* [AlFa], [GaZo].
Assuming $\gamma = 0$, $\beta = 1$ and $\alpha = 1/2$, the Lindblad operators L, L^*, become then the usual bosonic *creation-* and *anihilation-operators*

$$af(x) := (\frac{x}{2} + \partial_x)f(x), \quad a^*f(x) := (\frac{x}{2} - \partial_x)f(x), \tag{2.19}$$

which, in contrast to the corresponding *fermionic* creation- and anihilation-operators, are unbounded. Of course, all results in our work can be equivalently interpeted in this framework of second quantization.

Example 2.5. A particularly interesting example in the above class is the *Quantum Fokker-Planck equation* (QFP). As a PDE for the kernel $\rho(x, y, t) \in L^2(\mathbb{R}^{2d})$ it reads

$$\begin{aligned}\partial_t \rho = &- i\left(-\frac{\Delta_x}{2} + V(x,t) + \frac{\Delta_y}{2} - V(y,t)\right)\rho - \gamma(x-y)\cdot(\nabla_x - \nabla_y)\,\rho \\ &+ \left(D_{qq}|\nabla_x + \nabla_y|^2 - D_{pp}|x-y|^2 + 2iD_{pq}(x-y)\cdot(\nabla_x + \nabla_y)\right)\rho,\end{aligned} \tag{2.20}$$

subject to

$$\rho(x, y, t = 0) = \rho_0(x, y). \tag{2.21}$$

This model can be written in the form (2.10), (2.15), iff the conditions

$$D_{pp}D_{qq} - D_{pq}^2 \geq \frac{\gamma^2}{4}, \quad D_{pp}, D_{qq} \geq 0, \tag{2.22}$$

hold (see [ALMS] for more details and a particular choice of the parameters μ, α_j, β_j, $\gamma_j = 0$). The name Quantum Fokker-Planck equation stems from the fact that (2.20) can be transformed into the following kinetic equation

$$\begin{cases} \partial_t w + \xi \cdot \nabla_x w + \Theta[V]w = \mathcal{Q}w, & x, \xi \in \mathbb{R}^d, t > 0 \\ \qquad w\big|_{t=0} = w_0(x,\xi) & \end{cases} \tag{2.23}$$

using the *Wigner transform* [Wi], [LiPa]

$$w(x, \xi, t) := \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \rho\left(x + \frac{y}{2},\, x - \frac{y}{2}, t\right) e^{i\xi\cdot y}dy. \tag{2.24}$$

The diffusion operator $\mathcal{Q}$ in (2.23) is defined by

$$\mathcal{Q}w(x,\xi) := D_{pp}\Delta_\xi w + 2\gamma\,\mathrm{div}_\xi(\xi w) + D_{qq}\Delta_x w + 2D_{pq}\,\mathrm{div}_x(\nabla_\xi w). \tag{2.25}$$

Clearly, this is a generalization of the classical *kinetic Fokker-Planck operator* (FP), obtained by setting $D_{qq} = D_{pq} = 0$, *cf.* [Ri]. This case also corresponds

to the so called *Caldeira-Leggett* master equation [CaLe]. Note that for $\gamma > 0$, condition (2.22) implies that (2.25) is uniformly elliptic, which disqualifies the classical FP diffusion operator as an appropriate quantum mechanical equation. Nevertheless, it is sometimes used in applications as a phenomenological quantum model, *cf.* [St].
In (2.23), the pseudo-differential operator $\Theta[V]$, acting on the (not necessarily positive) phase space distribution w, is defined by

$$\Theta[V]w(x,\xi,t) := \frac{i}{(2\pi)^d} \int\int_{\mathbb{R}^d\times\mathbb{R}^d} \left[V\left(x+\frac{y}{2},t\right) - V\left(x-\frac{y}{2},t\right)\right] w(x,\xi',t)\; e^{iy\cdot(\xi-\xi')} d\xi' dy. \qquad (2.26)$$

First analytical results on the *Wigner-Fokker-Planck* equation (2.23) are in [SCDM] (linear equation, large-time behavior) and in [ALMS] (local-in-time solutions for the mean-field model). Equations of Quantum/Wigner-Fokker-Planck type play an important role within the areas of quantum optics (laser physics), quantum Brownian motion and the description of decoherence and diffusion of quantum states, *cf.* [De], [DGHP], [DHR], [Di], [Di1], [HuMa], [Va], [Va1] and the refernces given therein. The self-consistent Wigner-Poisson-Fokker-Planck systems is also used for semiconductor device simulations [St]. Indeed most of these models can be traced back to an early work by Feynman and Vernon [FeVe].
So far, however, a rigorous derivation of the QFP equation from many-body quantum mechanics is still missing. To the authors' knowledge, the only results in this direction are [CEFM], [FMR], where some special cases of the QFP equation are derived, using the Wigner formalism.
For more information on the rigoros derivation of Markovian master equations we refer to [Al], [Sp].

3 Existence of a conservative QDS for the linear problem

We consider the linear evolution problem on $\tilde{\mathcal{J}}_1$

$$\begin{cases} \dfrac{d}{dt}\rho = \mathcal{L}(\rho), \quad t>0, \\ \rho\big|_{t=0} = \rho_0 \in \mathcal{J}_1. \end{cases} \qquad (3.1)$$

Here, $\mathcal{L}(\rho) := -i\,[H,\rho] + A(\rho)$ is the formal generator of a QDS on $\tilde{\mathcal{J}}_1$, with

$$H = -\frac{\Delta}{2} + \frac{|x|^2}{2} + V_1(x) - i\mu[x,\nabla]_+. \qquad (3.2)$$

Definition 3.1. Given any Hilbert space $\mathcal{H}$, one defines a *conservative quantum dynamical semigroup* (QDS) as a one parameter C_0 - semigroup of bounded operators

$$\Phi_t : \mathcal{J}_1(\mathcal{H}) \to \mathcal{J}_1(\mathcal{H}), \qquad (3.3)$$

which in addition satisfies:

(a) The dual map $\Phi_t^* : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$, defined by

$$\mathrm{Tr}(A\Phi_t(\rho)) = \mathrm{Tr}(\Phi_t^*(A)\rho), \tag{3.4}$$

for all $\rho \in \mathcal{J}_1(\mathcal{H})$, $A \in \mathcal{B}(\mathcal{H})$, is *completely positive.* This means that the map

$$\Phi_t^* \otimes \mathrm{I}_n : \mathcal{B}(\mathcal{H}) \otimes \mathcal{B}(\mathcal{H}_n) \to \mathcal{B}(\mathcal{H}) \otimes \mathcal{B}(\mathcal{H}_n) \tag{3.5}$$

is positive (*i.e.* positivity preserving) for all $n \in \mathbb{N}$. Here $\mathcal{H}_n$ denotes a finite dimensional Hilbert space and I_n is the $n-$ *dimensional* unit matrix.

(b) Φ_t is trace preserving, *i.e.* conservative (or unital).

Remark 3.2. The notion QDS is sometimes reserved for the dual semigroup Φ_t^*. Physically speaking, this corresponds to the *Heisenberg picture.* The appropriate continuity is then

$$\lim_{t\to 0} \mathrm{Tr}(\rho(\Phi_t^*(A) - A)) = 0, \tag{3.6}$$

for all $\rho \in \mathcal{J}_1(\mathcal{H})$, $A \in \mathcal{B}(\mathcal{H})$, *i.e. ultraweak continuity.* Complete positivity can be defined also for operators on general C^*-Algebras $\mathcal{A}$ [Sti] and it is known that complete positivity and positivity are equivalent only if $\mathcal{A}$ is commutative. (Counter-examples can be found already for 2×2 complex valued matrices, see *e.g.* [AlFa].) Again, from a physical point of view, complete positivity can be interpreted as preservation of positivity under *entanglement.*

Following the classical work of Davies [Da1] we shall start to investigate the properties of the operator

$$Y := -iH - \frac{1}{2}L. \tag{3.7}$$

First we need the following technical lemma, the proof of which introduces some important notations used throughout this work.

Lemma 3.3. *Let $P := p_2(x, -i\nabla)$ be a linear operator on $L^2(\mathbb{R}^d)$ over the field $\mathbb{C}$, where p_2 is a complex valued, quadratic polynomial and specify its domain by*

$$\mathcal{D}(P) := \{f : \mathrm{Re}\, f, \mathrm{Im}\, f \in C_0^\infty(\mathbb{R}^d)\}. \tag{3.8}$$

Then $\overline{P}$ is the maximal extension of P in the sense that

$$\mathcal{D}(\overline{P}) = \{f \in L^2(\mathbb{R}^d) : \textit{the distribution } Pf \in L^2(\mathbb{R}^d)\}. \tag{3.9}$$

Proof. (sketch) Let us define a mollifying delta sequence by

$$\varphi_n(x) := n^d \varphi(nx), \quad x \in \mathbb{R}^d, n \in \mathbb{N}, \tag{3.10}$$

and assume that

$$\varphi \in C_0^\infty,\ \varphi \geq 0,\ \varphi(x) = \varphi(-x),\ \int_{\mathbb{R}^d} \varphi(x)dx = 1,\ \mathrm{supp}\,\varphi \subset \{|x| < 1\}.$$

Also, a sequence of radially symmetric cutoff function is defined by

$$\chi_n(x) := \chi\left(\frac{|x|}{n}\right), \quad x \in \mathbb{R}^d, n \in \mathbb{N}, \tag{3.11}$$

such that it fulfills for all $x \in \mathbb{R}^d$

$$\chi_n \in C_0^\infty,\ 0 \le \chi \le 1,\ \operatorname{supp} \chi \subset [0,1],\ \chi\Big|_{[0,\frac{1}{2}]} \equiv 1 \quad .$$

In the sequel we shall use the resulting bounds

$$|\chi^{(m)}(x)| \le K_m,\ m \in \mathbb{N}.$$

We define an approximating sequence for $f \in L^2(\mathbb{R}^d)$, by

$$f_n(x) := \chi_n(x)(f * \varphi_n)(x), \quad n \in \mathbb{N}. \tag{3.12}$$

Clearly, $f_n \in \mathcal{D}(P)$ by construction. We have to prove that for all $f \in L^2(\mathbb{R}^d)$, with $Pf \in L^2(\mathbb{R}^d)$, $f_n \to f$ in the graph norm $\|f\|_P := \|f\|_2 + \|Pf\|_2$. Because $\varphi_n \to \delta$ in $\mathcal{D}'(\mathbb{R}^d)$ (the space of distributions) and $\chi_n \to 1$ pointwise, we clearly have

$$f_n \overset{n\to\infty}{\longrightarrow} f \text{ in } L^2(\mathbb{R}^d). \tag{3.13}$$

The remainder of the proof, *i.e.* $Pf_n \to Pf$ in $L^2(\mathbb{R}^d)$, is now analogous to the proof of lemma 2.2 in [ACD], when extended to complex valued functions f. A similar strategy is used again in the proof of lemma 3.7 below. □

Remark 3.4. Lemma 3.3 asserts that the *minimal* and *maximal operators* defined by the expression $P = p_2(x, -i\nabla)$ coincide. This fact is closely related to the essential self-adjointness of Schrödinger operators, cf. §2.8.6 in [EgSh]. The lemma provides an elementary proof of the well known fact that the Hamiltonian $H = -\Delta - |x|^2$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^d)$, cf. [Ka], Corollary to Theorem X.38 in [ReSi2]; – just apply the lemma to H with $\mathcal{D}(H) = C_0^\infty(\mathbb{R}^d)$ and to $H^*\Big|_{\mathcal{D}(H)}$. On the other hand, it is well known that $H = -\Delta + x^2 - x^4$ is *not* essentially self-adjoint on $C_0^\infty(\mathbb{R})$, cf. Example 1 of X.5 in [ReSi2]. Therefore, lemma 3.3 can, in general, *not* be extended to higher order polynomials $p(x, -i\nabla)$.
This can be further illustrated by the following example, *cf.* [CGQ]: Consider the third-order symmetric operator $H = i((1 + x^2)\partial_x + \partial_x(1 + x^2))$ on $C_0^\infty(\mathbb{R})$. Then H is not essentialy self-adjoint, since one can easily check that there exists a nontrivial eigenvector corresponding to the eigenvalue $-i$. Thus the above lemma can not be extended to this case either.

With the above lemma we can now prove that the main technical assumption on the operator Y (imposed in [Da1], [ChFa]) is fulfilled.

Proposition 3.5. *Let $V_1 = 0$ and let the operator Y be defined on*

$$\mathcal{D}(Y) := \{f \in L^2(\mathbb{R}^d) : \Delta f, |x|^2 f \in L^2(\mathbb{R}^d)\}. \tag{3.14}$$

(a) *Then its closure $\overline{Y}$ is the infinitesimal generator of a C_0 - contraction semigroup on $L^2(\mathbb{R}^d)$.*
(b) *Further, the operators L_j, $L_j^* : \mathcal{D}(\overline{Y}) \to L^2(\mathbb{R}^d)$ satisfy*

$$\langle Yf, g\rangle + \langle f, Yg\rangle + \sum_{j=1}^{M} \langle L_j f, L_j g\rangle = 0, \quad \forall f, g \in \mathcal{D}(\overline{Y}), \tag{3.15}$$

where $\langle\cdot,\cdot\rangle$ denotes the standard scalar product on $L^2(\mathbb{R}^d)$.

Proof. First note that for $f \in \mathcal{D}(Y)$ the term $x \cdot \nabla f$, which appears in Yf, is also in $L^2(\mathbb{R}^d)$. This can be obtained by an interpolation argument. Further, $\mathcal{D}(Y)$ is dense in $L^2(\mathbb{R}^d)$, since $C_0^\infty(\mathbb{R}^d)$ is. By Lemma 3.3 we have

$$\mathcal{D}(\overline{Y}) = \{f \in L^2(\mathbb{R}^d) : Yf \in L^2(\mathbb{R}^d)\}.$$

Part (a): The proof proceeds in several steps:
Step 1: We study the dissipativity of Y, which in our case is defined by

$$\mathrm{Re}\,\langle Yf, f\rangle \leq 0, \quad \forall f \in \mathcal{D}(Y).$$

Since H from (3.7) is symmetric we obtain

$$\mathrm{Re}\,\langle iHf, f\rangle = 0, \quad \forall f \in \mathcal{D}(Y).$$

Also we get

$$-\,\mathrm{Re}\left\langle L_j^* L_j f, f\right\rangle = -\left\langle L_j f, L_j f\right\rangle \leq 0, \quad \forall f \in \mathcal{D}(Y).$$

Thus Y is dissipative and by theorem 1.4.5b of [Pa] also its closure $\overline{Y}$ is.
Step 2: Its adjoint is $Y^* = iH - \frac{1}{2}L$, with domain of definition $\mathcal{D}(Y^*)$. We have $\mathcal{D}(Y^*) \supseteq \mathcal{D}(Y)$, since

$$\langle Yf, g\rangle = \langle f, Y^* g\rangle\,, \quad \forall f, g \in \mathcal{D}(Y).$$

As in step 1 we conclude that $Y^*\Big|_{\mathcal{D}(Y)}$ is dissipative. We can now apply lemma 3.3 to $P = Y^*\Big|_{\mathcal{D}(P)}$ with $\mathcal{D}(P)$ defined in (3.8). Then P is dissipative on $\mathcal{D}(P) \subseteq \mathcal{D}(Y) \subseteq \mathcal{D}(Y^*)$. Since Y^* is closed, we have $\mathcal{D}(Y^*) = \mathcal{D}(\overline{P})$, the domain of the maximal extension. Thus Y^* is dissipative on all of $D(Y^*)$.
Step 3: Application of the Lumer-Phillips theorem (corollary 1.4.4 in [Pa]) to $\overline{Y}$ (with $(\overline{Y})^* = Y^*$) implies the assertion.
Part (b): We need to show: If $f, Yf \in L^2(\mathbb{R}^d)$, then $L_j f$, $L_j^* f \in L^2(\mathbb{R}^d)$ follows. This can be easily seen from the fact that

$$\frac{1}{2}\sum_j \langle L_j f, L_j f\rangle = -\,\mathrm{Re}\,\langle Yf, f\rangle < \infty.$$

Equation (3.15) is then obtained by a simple computation. □

With these properties of $\overline{Y}$ (as stated in proposition 3.5), theorem 3.1 of [Da1] asserts that (3.1) has a so called *minimal solution*:

Proposition 3.6. [Davies '77] *There exists a positive C_0 - semigroup of contractions Φ_t on $\tilde{\mathcal{J}}_1$. Its infinitesimal generator is the evolution operator $\mathcal{L}$, defined on a sufficiently large domain $\mathcal{D}(\mathcal{L})$, such that $\tilde{\mathcal{J}}_1 \supseteq \mathcal{D}(\mathcal{L}) \supseteq \mathcal{D}(Z)$.*
Here, $Z : \mathcal{D}(Z) \to \tilde{\mathcal{J}}_1$ is the maximally extended operator with domain

$$\mathcal{D}(Z) = \{\rho \in \tilde{\mathcal{J}}_1(L^2(\mathbb{R}^d)) : Z(\rho) := Y\rho + \rho Y^* \in \tilde{\mathcal{J}}_1(L^2(\mathbb{R}^d))\}. \tag{3.16}$$

From the above proposition we learn that the formal generator $\mathcal{L}$, in general, does not unambiguously define a solution of the corresponding master equation,

in the sense of semigroups. Also, it is well known, that the obtained minimal solution need not be trace preserving (for nonconservative examples see *e.g.* [Da1], [Ho], [Qu]).
On the other hand, if the semigroup corresponding to the minimal solution preserves the trace, it is the unique conservative QDS associated to the abstract evolution problem (3.1), *cf.* [CGQ], [ChFa], [FaRe], [Ho]. This situation is similar to the one for the Kolmogorov-Feller differential equations appearing in the theory of Markov processes [Fe].
We are going to prove now that in our case the minimal solution is indeed the unique QDS. To this end, we need to introduce some more notation:
From now on we denote by

$$(M(g)f)(x) := g(x)f(x), \quad (C(g)f)(x) := (g * f)(x), \quad g \in C_0^\infty(\mathbb{R}^d),$$

a family of multiplication and convolution operators on $L^2(\mathbb{R}^d)$, where " $*$ " is the usual convolution w.r.t. x. Further we define, for $n \in \mathbb{N}$, a family of sets $\mathcal{D}_n \subset \tilde{\mathcal{J}}_1(L^2(\mathbb{R}^d))$ by

$$\mathcal{D}_n := \{\sigma_n \in \tilde{\mathcal{J}}_1 : \exists \rho \in \tilde{\mathcal{J}}_1 \ s.t. \ \sigma_n = M(\chi_n)C(\varphi_n)\rho \, C(\varphi_n)M(\chi_n)\}, \tag{3.17}$$

where χ_n, φ_n are the cutoff resp. mollifying functions defined in the proof of lemma 3.3 above. For an operator $\rho \geq 0$ with kernel (2.6), the operator σ_n has an integral kernel given by

$$\begin{aligned} \sigma_n(x,y) = \ & \chi_n(x)\varphi_n(x) \underset{x}{*} \rho(x,y) \underset{y}{*} \varphi_n(y)\chi_n(y) \\ = \ & \sum_{j\in\mathbb{N}} \lambda_j \ \varphi_{j,n}(x) \ \overline{\varphi_{j,n}(y)}, \end{aligned} \tag{3.18}$$

where $\varphi_{j,n}(x) := \chi_n(x)(\varphi_n * \psi_j)(x) \in C_0^\infty(\mathbb{R}^d)$ and $\|\varphi_{j,n}\|_2 \leq \|\psi_j\|_2 = 1$. Since $\sigma_n \geq 0$ we get

$$|||\sigma_n|||_1 = \operatorname{Tr} \sigma_n = \sum_{j\in\mathbb{N}} \lambda_j \|\varphi_{j,n}\|_2^2 \leq \sum_{j\in\mathbb{N}} \lambda_j = |||\rho|||_1. \tag{3.19}$$

The unit of all sets $\mathcal{D}_n$ will be denoted by

$$\mathcal{D}_\infty := \bigcup_{n\in\mathbb{N}} \mathcal{D}_n. \tag{3.20}$$

Also we shall write for the graph norm corresponding to $\mathcal{L}$

$$\|\rho\|_{\mathcal{L}} := |||\rho|||_1 + |||\mathcal{L}(\rho)|||_1. \tag{3.21}$$

Then the following technical result, which is a key point in the existence and uniqueness analysis, holds.

Lemma 3.7. *Let $V_1 = 0$. Then:*
(a) *The set $\mathcal{D}_\infty$ is dense in $\tilde{\mathcal{J}}_1$.*
(b) $\mathcal{D}_\infty \subset \mathcal{D}(Z) \subset \mathcal{D}(\mathcal{L})$.
(c) *The operator $\overline{\mathcal{L}\,|_{\mathcal{D}_\infty}}$ is the maximal extension of $\mathcal{L}$, in the sense that for each $\rho \in \tilde{\mathcal{J}}_1$, with $\mathcal{L}(\rho) \in \tilde{\mathcal{J}}_1$, there exists a sequence $\{\sigma_n\}_{n\in\mathbb{N}} \subset \mathcal{D}_\infty$, such that*

$$\lim_{n\to\infty} \|\rho - \sigma_n\|_{\mathcal{L}} = 0. \tag{3.22}$$

Proof. The proof is deferred to the appendix. □

Remark 3.8. For all $\rho \in \tilde{\mathcal{J}}_1$, $\mathcal{L}(\rho)$ can be defined (at least) as an operator $\mathcal{L}(\rho) : C_0^\infty(\mathbb{R}^d) \to \mathcal{D}'(\mathbb{R}^d)$, the space of distributions. For $\mathcal{L}(\rho) \in \tilde{\mathcal{J}}_1$ to hold, first of all an appropriate extension has to exist, such that $\mathcal{L}(\rho) \in \mathcal{B}(L^2(\mathbb{R}^d))$.

We are now in the position to state our first main theorem:

Theorem 3.9. *Let $V_1 = 0$. The evolution operator $\mathcal{L}$ generates on $\tilde{\mathcal{J}}_1$ a conservative quantum dynamical semigroup of contractions $\Phi_t(\rho) = e^{\mathcal{L}t}\rho$. This QDS yields the unique mild solution, in the sense of semigroups, for the abstract evolution problem (3.1).*

Proof. Existence of $\Phi_t(\rho) = e^{\mathcal{L}t}\rho$ is guaranteed by proposition 3.6. As a semigroup generator $\mathcal{L}$ is closed, and by lemma 3.7 it is the maximally extended evolution operator. This implies uniqueness of the semigroup. Complete positivity then follows from Stinespring's theorem [Sti], [AlFa].

It remains to prove the conservativity for the obtained QDS. This will be done by using a similar argument as in the proof of theorem 3.2 in [Da1]:

Step 1: For the special case $\rho_0 \in \mathcal{D}(\mathcal{L})$ the trajectory $\Phi_t(\rho_0)$ is a classical solution (in the sense of semigroups, *cf.* [Pa]), *i.e.* $\Phi_t(\rho_0) \in C^1([0,\infty), \mathcal{J}_1(L^2(\mathbb{R}^d)))$ and $\Phi_t(\rho_0) \in \mathcal{D}(\mathcal{L})$, $\forall\, t \geq 0$. Hence $\operatorname{Tr} \Phi_t(\rho_0) \in C^1([0,\infty), \mathbb{R})$ and we calculate for $t \geq 0$:

$$\frac{d}{dt} \operatorname{Tr} \Phi_t(\rho_0) = \operatorname{Tr} \frac{d}{dt} \Phi_t(\rho_0) = \operatorname{Tr} \mathcal{L}(\Phi_t(\rho_0)) = 0. \tag{3.23}$$

To justify the last equality we note that $\mathcal{D}_\infty$ is $\|\cdot\|_{\mathcal{L}}$ - dense in $\mathcal{D}(\mathcal{L})$, by lemma 3.7 (c). Thus we can approximate $\Phi_t(\rho_0)$, for every fixed $t \geq 0$, by an appropriate sequence $\{\sigma_n\} \subseteq \mathcal{D}_\infty$. Since $\mathcal{D}_\infty$ is included in the domain of each "term" (A.1) of the operator $\mathcal{L}$ (as the proof of lemma 3.7 (b) shows), the cyclicity of the trace yields $\operatorname{Tr} \mathcal{L}(\Phi_t(\rho_0)) = 0$. Equation (3.23) then implies

$$\operatorname{Tr} \Phi_t(\rho_0) = \operatorname{Tr} \rho_0 = 0, \quad \forall \rho_0 \in \mathcal{D}(\mathcal{L}), t \geq 0.$$

Step 2: The general case $\rho_0 \in \tilde{\mathcal{J}}_1(L^2(\mathbb{R}^d))$ (*i.e.* $\Phi_t(\rho_0)$ is a mild solution) follows from step 1 and the fact that $\mathcal{D}(\mathcal{L})$ is dense in $\tilde{\mathcal{J}}_1(L^2(\mathbb{R}^d))$. □

From the above theorem, we obtain the the following corollary:

Corollary 3.10. *For $\rho \in \mathcal{D}(\mathcal{L})$ let*

$$\tilde{\mathcal{L}}(\rho) := \mathcal{L}(\rho) + \mathcal{L}_p(\rho), \tag{3.24}$$

where

$$\mathcal{L}_p(\rho) := -i[V_1, \rho] + \sum_{j=M+1}^{\infty} L_j \rho L_j^* - \frac{1}{2}\left[L_j^* L_j, \rho\right]_+, \tag{3.25}$$

with $V_1 \in L^\infty(\mathbb{R}^d)$, $L_j \in \mathcal{B}(L^2(\mathbb{R}^d))$ and the sum converges in $\mathcal{B}(\tilde{\mathcal{J}}_1(L^2(\mathbb{R}^d)))$. Then the perturbed operator $\tilde{\mathcal{L}}$ again uniquely defines a conservative QDS of contractions.

Proof. Existence and uniqueness of the C_0-semigroup follows from standard perturbation results, *cf.* [Pa]. To prove conservativity of the perturbed QDS, let $\rho(t)$ denote the solution of

$$\frac{d}{dt}\rho = \tilde{\mathcal{L}}(\rho), \quad \rho(0) = \rho_0.$$

The conservativity then follows from Duhamel's representation

$$\rho(t) = \Phi_t(\rho_0) + \int_0^t \Phi_{t-s}(\mathcal{L}_p(\rho(s)))\, ds, \tag{3.26}$$

by noting that $\mathrm{Tr}(\mathcal{L}_p(\rho)) = 0$. All other properties can be established by the same procedure as in theorem 1 of [AlMe] or by a Picard iteration. □

Remark 3.11. An alternative approach to prove theorem (3.9) could be to verify the sufficient conditions of [ChFa]. In fact their assumptions A1 and A2 are simple consequences of our lemma (3.3) and proposition (3.5). For their third condition A3 however, one would need to prove that $C_0^\infty(\mathbb{R}^d)$ is a core for Y^2, defined on

$$\mathcal{D}(Y^2) := \{f \in \mathcal{D}(\overline{Y}) : \overline{Y}f \in \mathcal{D}(\overline{Y})\}. \tag{3.27}$$

With considerable more effort, the proof should be possible by extending the strategy of lemma (3.3). However, one can expect quite cumbersome calculations.

4 Local-in-time existence of the mean field QDS

We shall now prove existence and uniqueness of local-in-time solutions for the nonlinear evolution problem

$$\begin{cases} \dfrac{d}{dt}\rho = \mathcal{L}(\rho), \quad t > 0 \\ \rho(0) = \rho_0 \in \tilde{\mathcal{J}}_1. \end{cases} \tag{4.1}$$

Here, the nonlinear map $\mathcal{L}$ is given by

$$\mathcal{L}(\rho) := -i\left[-\frac{\Delta}{2} + V[\rho] - i\mu[x,\nabla]_+, \rho\right] + A(\rho), \tag{4.2}$$

where the self-consistent potential $V[\rho]$ is given as in (2.12) and $A(\rho)$ is the Lindblad operator defined by (2.15) and (2.17).

To this end, we shall prove that the linear evolution problem (3.1) not only defines a C_0-semigroup in $\tilde{\mathcal{J}}_1$ (guaranteed by theorem (3.9)) but also in an appropriate energy space. This is a parallel procedure (apart from severe technical difficulties) to solving the *Schrödinger-Poisson* equation in $H^1(\mathbb{R}^d)$, *cf.* [GiVe]. Note that Davies' construction of a minimal QDS is valid *only* in $\mathcal{J}_1$. Hence, the required additional regularity of $\Phi_t(\rho_0)$ has to be established explicitly. Also, one has to prove seperately that this nonlinear model conserves the positivity and the trace of ρ.

In the following, we shall restrict ourselves to the physical most important case of $d = 3$ spatial dimensions.

Let us start by introducing the following definitions:

Definition 4.1. The *kinetic energy* of a density matrix operator $\rho \in \tilde{\mathcal{J}}_1$ is defined by

$$E^{kin}[\rho] := \frac{1}{2}\,\mathrm{Tr}(\sqrt{-\Delta}\,|\rho|\sqrt{-\Delta}) \geq 0, \tag{4.3}$$

where $\sqrt{-\Delta}$ denotes a *pseudo-differential operator* with symbol $|\xi|$, $\xi \in \mathbb{R}^d$, *i.e.*

$$\sqrt{-\Delta} f(x) := \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} |\xi|(\mathcal{F}f)(\xi)e^{i\xi\cdot x}d\xi, \quad \forall f \in H^1(\mathbb{R}^d). \tag{4.4}$$

Further, we define the *external* and the *self-consistent potential energy* of $\rho \in \tilde{\mathcal{J}}_1$ by

$$E^{ext}[\rho] := \frac{1}{2}\,\mathrm{Tr}(|x|\,|\rho|\,|x|) \geq 0, \quad E^{sc}[\rho] := \frac{1}{2}\,\mathrm{Tr}(\phi[\rho]\rho). \tag{4.5}$$

The total energy will be denoted by

$$E^{tot}[\rho] := E^{kin}[\rho] + E^{ext}[\rho] + E^{sc}[\rho]. \tag{4.6}$$

In the sequel we shall work in the following energy space $\mathcal{E}$:

$$\mathcal{E} := \{\rho \in \tilde{\mathcal{J}}_1 : \sqrt{-\Delta}\,|\rho|\sqrt{-\Delta}, |x|\,|\rho|\,|x| \in \mathcal{J}_1\}, \tag{4.7}$$

equipped with the norm

$$\|\rho\|_{\mathcal{E}} := |||\,\rho\,|||_1 + |||\sqrt{-\Delta}\,|\rho|\sqrt{-\Delta}|||_1 + |||\,|x|\,\rho\,|x|\,|||_1. \tag{4.8}$$

Note the additional factor $1/2$ in front of the term $E^{sc}[\rho]$, which does not appear in the Hamiltonian (2.11), (2.12). It is due to the self-consistent nonlinearity, *cf.* [Ar]. For *physical* states we have $\rho \geq 0$, from which we easily get $E^{sc}[\rho] \geq 0$, since $\rho \geq 0$ implies $n[\rho] \geq 0$ and hence $\phi[\rho] \geq 0$, by (2.14).
Further note that in this defintions we neglected the term $-i\mu[x, \nabla]_+$, which appears in the generalized (or adjusted) Hamiltonian operator (2.11) of our system. Thus, even in the linear case, we have $E^{tot}[\rho] \neq \mathrm{Tr}(H\rho)$. The latter term would be the more common definition for the energy of the system. We note that we shall use $E^{tot}[\rho]$ only for deriving a-priori estimates and towards this end $E^{tot}[\rho]$ is the more convenient expression.

Remark 4.2. Using the cyclicity of the trace, one formally obtains the more common expression for the kinetic energy of a physical state $\rho \geq 0$:

$$E^{kin}[\rho] := \frac{1}{2}\,\mathrm{Tr}(\sqrt{-\Delta}\,\rho\sqrt{-\Delta}) = \frac{1}{2}\,\mathrm{Tr}(-\Delta\rho). \tag{4.9}$$

However, these two expressions for $E^{kin}[\rho]$ are not fully equivalent, since $\Delta\rho \in \tilde{\mathcal{J}}_1$ requires more regularity on ρ than just requiring $\sqrt{-\Delta}\rho\sqrt{-\Delta} \in \tilde{\mathcal{J}}_1$. (For more details see *e.g.* [Ar] and the references given therein.) We further remark that if the kernel of ρ is given as in (2.6) the kinetic energy reads

$$E^{kin}[\rho] = \frac{1}{2}\sum_{j\in\mathbb{N}} \lambda_j\ \|\nabla\psi_j\|_2^2 \geq 0. \tag{4.10}$$

Using these definitions, we will now prove that the sum of kinetic and (external) potential energy is continuous in time during the linear evolution.

Lemma 4.3. *Let $V_1 = 0$ and $\rho_0 \in \mathcal{E}$, then*

$$(E^{kin} + E^{ext})[\rho(t)] \in C([0,\infty);\mathbb{R}), \tag{4.11}$$

where $\rho(t) := \Phi_t(\rho_0) \in C([0,\infty), \tilde{\mathcal{J}}_1)$ denotes the unique QDS for the linear evolution problem, given by (3.1).

Proof. The idea of the proof is to derive a differential inequality for $E^{kin} + E^{ext}$ from (3.1). First, we note that each $\rho_0 \in \mathcal{E} \subset \tilde{\mathcal{J}}_1$ can be uniquely decomposed into its positive and negative part: $\rho_0 = \rho_0^+ - \rho_0^-$, with $\rho_0^\pm \geq 0$, *cf.* [ReSi1]. Since Φ_t preserves positivity, we can restrict ourselves in the following to the case $\rho_0 \geq 0$ and hence $\rho(t) \geq 0$.
Let us define some energy functionals for positive $\rho \in \tilde{\mathcal{J}}_1$:

$$E_{k,l}^{kin}[\rho] := -\frac{1}{2}\operatorname{Tr}(\partial_k \rho \partial_l), \quad E_{k,l}^{ext}[\rho] := \frac{1}{2}\operatorname{Tr}(x_k \rho x_l), \tag{4.12}$$

with $k,l = 1,\dots,d$. For $\rho \in \mathcal{D}_\infty$, the cyclicity of the trace implies

$$E^{kin}[\rho] = \sum_{k=1}^{d} E_{k,k}^{kin}[\rho], \quad E^{ext}[\rho] = \sum_{k=1}^{d} E_{k,k}^{ext}[\rho] \tag{4.13}$$

and, by a density argument, the formulas (4.13) also hold for $\rho \in \mathcal{E}$.
Step 1: We apply the operators x_k, ∂_k (from left and right) to (3.1) and take traces. A lengthy but straightforward calculation, using the cyclicity of the trace and setting w.r.o.g. $\operatorname{Tr}\rho(t) = 1$, yields for the kinetic energy:

$$\begin{aligned}\sum_{k=1}^{d} \frac{d}{dt} E_{k,k}^{kin} &= \frac{1}{2}\sum_{k=1}^{d}\sum_{j=1}^{M} |\alpha_{j,k}|^2 - 4\mu \sum_{k=1}^{d} E_{k,k}^{kin} - 2\sum_{k,l=1}^{d}\sum_{j=1}^{M} \operatorname{Re}(\alpha_{j,k}\overline{\beta_{j,l}}) E_{k,l}^{kin} \\ &\quad - \sum_{k,l=1}^{d} i \sum_{j=1}^{M} \operatorname{Im}(\alpha_{j,k}\overline{\alpha_{j,l}}) \operatorname{Tr}(\partial_k \rho x_l) + \operatorname{Im}(\alpha_{j,k}\overline{\gamma_j}) \operatorname{Tr}(\rho \partial_k) \\ &\quad + i\left(\frac{d}{2} + \sum_{k=1}^{d} \operatorname{Tr}(\partial_k \rho x_k)\right).\end{aligned} \tag{4.14}$$

For the external energy we obtain:

$$\begin{aligned}\sum_{k=1}^{d} \frac{d}{dt} E_{k,k}^{ext} &= -\frac{1}{2}\sum_{k=1}^{d}\sum_{j=1}^{M} |\beta_{j,k}|^2 + 4\mu \sum_{k=1}^{d} E_{k,k}^{ext} + 2\sum_{k,l=1}^{d}\sum_{j=1}^{M} \operatorname{Re}(\alpha_{j,k}\overline{\beta_{j,l}}) E_{k,l}^{ext} \\ &\quad + i \sum_{k,l=1}^{d} \sum_{j=1}^{M} \operatorname{Im}(\beta_{j,k}\overline{\beta_{j,l}}) \operatorname{Tr}(\partial_k \rho x_l) + \operatorname{Im}(\beta_{j,k}\overline{\gamma_j}) \operatorname{Tr}(\rho x_k) \\ &\quad - i\left(\frac{d}{2} + \sum_{k=1}^{d} \operatorname{Tr}(\partial_k \rho x_k)\right).\end{aligned} \tag{4.15}$$

Step 2: These equations are not closed in E^{kin} and E^{ext}. To circumvent this problem, we shall use interpolation arguments: First, note that $(\partial_k \rho \partial_k) \in \mathcal{J}_1$, iff $(\partial_k \sqrt{\rho}) \in \mathcal{J}_2$, *cf.* [ReSi1]. Thus we can estimate

$$|||\rho \partial_k|||_1^2 \leq |||\sqrt{\rho}|||_2^2 \; |||\sqrt{\rho}\partial_k|||_2^2 = |||\rho|||_1 \; |||\partial_k \rho \partial_k|||_1.$$

Likewise, we get

$$|||\partial_k \rho x_l|||_1^2 \leq \; |||\partial_k \sqrt{\rho}|||_2^2 \; |||\sqrt{\rho} x_l|||_2^2 \; = \; |||\partial_k \rho \partial_k|||_1 \; |||x_l \rho x_l|||_1$$

and one easily derives analogous estimates for the off-diagonal energy-terms $E_{k,l}^{ext/kin}$. Hence, estimating term-by-term in (4.14), (4.15), we finally obtain

$$\left| \frac{d}{dt} \sum_{k=1}^{d} (E_{k,k}^{kin} + E_{k,k}^{ext})[\rho(t)] \right| \leq \; K \sum_{k=1}^{d} (E_{k,k}^{kin} + E_{k,k}^{ext})[\rho(t)],$$

with some generic constant $K \geq 0$. Applying Gronwall's lemma then gives the desired result. □

This lemma directly leads to our next proposition:

Proposition 4.4. *Assume that $\rho_0 \in \mathcal{E}$ and $V_1 \in L^\infty(\mathbb{R}^d)$ s.t. additionally $\nabla V_1 \in L^q(\mathbb{R}^d)$, for some $3 \leq q \leq \infty$. Then*

$$\Phi_t(\rho_0) \in C([0,\infty), \mathcal{E}), \quad \forall t > 0, \tag{4.16}$$

where $\Phi_t(\rho_0)$ denotes the unique linear QDS corresponding to (3.1).

Proof. The proof is based on a generalization of Grümm's theorem. As in the proof of lemma 4.3 above, we only consider, w.r.o.g., the case $\rho(t) \geq 0$.
Step 1: At first, we shall prove that for all f, $g \in L^2(\mathbb{R}^d)$ and $s \geq 0$,

$$\begin{aligned} \lim_{t \to s} \langle f, \sqrt{-\Delta} \rho(t) \sqrt{-\Delta} g\rangle + \langle f, |x| \rho(t) |x| g\rangle = \langle f, \sqrt{-\Delta} \rho(s) \sqrt{-\Delta} g\rangle \\ + \langle f, |x| \rho(s) |x| g\rangle, \end{aligned} \tag{4.17}$$

where $\langle \cdot, \cdot \rangle$ denotes the standard $L^2(\mathbb{R}^d)$ scalar product.
To this end we choose two sequences $\{f_n\}$, $\{g_n\} \in H^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d; (1+|x|^2)dx)$, $n \in \mathbb{N}$, s.t. $f_n \overset{n\to\infty}{\longrightarrow} f$, $g_n \overset{n\to\infty}{\longrightarrow} g$ in $L^2(\mathbb{R}^d)$ and write

$$\begin{aligned} \langle f, \sqrt{-\Delta}\, (\rho(t) - \rho(s)) \sqrt{-\Delta}\, g\rangle &= \langle f_n, \sqrt{-\Delta}\, (\rho(t) - \rho(s)) \sqrt{-\Delta}\, g_n\rangle \\ &+ \langle f_n, \sqrt{-\Delta}\, (\rho(t) - \rho(s)) \sqrt{-\Delta}\, (g - g_n)\rangle \\ &+ \langle f - f_n, \sqrt{-\Delta}\, (\rho(t) - \rho(s)) \sqrt{-\Delta}\, g\rangle. \end{aligned} \tag{4.18}$$

Since $\rho(t) \in \mathcal{E}_+$ we have $|||\sqrt{-\Delta} \rho(t) \sqrt{-\Delta}|||_\infty \leq K$, for all $|t - s| < t_0$ and thus we can estimate for $n \in \mathbb{N}$ large enough:

$$\begin{aligned} \left| \langle f - f_n, \sqrt{-\Delta}\, (\rho(t) - \rho(s)) \sqrt{-\Delta}\, g\rangle \right| &\leq K \|f - f_n\|_2 \; \|g\|_2, \\ \left| \langle f_n, \sqrt{-\Delta}\, (\rho(t) - \rho(s)) \sqrt{-\Delta}\, (g - g_n)\rangle \right| &\leq K \|g - g_n\|_2 \; \|f_n\|_2. \end{aligned}$$

Now choose an arbitrary $\varepsilon \in \mathbb{R}_+$ and then $m \in \mathbb{N}$ large enough, such that for all $n > m$

$$\|f - f_n\|_2 \leq \frac{\varepsilon}{3K\|g\|_2}, \quad \|g - g_n\|_2 \leq \frac{\varepsilon}{6K\|f\|_2} \leq \frac{\varepsilon}{3K\|f_n\|_2}.$$

Since this choice is independent of t the second and the third term on the r.h.s. of (4.18) are smaller than $\varepsilon/3$.

By assumption, we have $\sqrt{-\Delta} f_n,\ \sqrt{-\Delta} g_n \in L^2(\mathbb{R}^d)$ and thus

$$\lim_{t\to s}\langle f_n, \sqrt{-\Delta}\,(\rho(t)-\rho(s))\sqrt{-\Delta}\,g_n\rangle = \lim_{t\to s}\langle \sqrt{-\Delta}\,f_n, (\rho(t)-\rho(s))\sqrt{-\Delta}\,g_n\rangle$$
$$= 0,$$

where the last equality follows from the fact that $\rho(t) \in C([0,\infty), \tilde{\mathcal{J}}_1)$ (by theorem 3.9). In other words

$$\langle f_n, \sqrt{-\Delta}(\rho(t)-\rho(s))\sqrt{-\Delta} g_n\rangle \le \frac{\varepsilon}{3},$$

for $|t-s|$ small enough. Since ε was arbitrary, equation (4.17) is true and it states that

$$\sqrt{-\Delta}\,\rho(t)\sqrt{-\Delta} \stackrel{t\to s}{\longrightarrow} \sqrt{-\Delta}\,\rho(s)\sqrt{-\Delta}\,,$$

in the weak operator topology.

Having in mind that $\rho(t) \in \mathcal{E}$ also implies $|||\ |x|\rho(t)|x|\ |||_\infty \le K$, exactly the same procedure can be applied to the second term of (4.17) and the assertion is proved.

Step 2: Let $V_1 = 0$ first. By theorem 2.20 in [Si] (a generalization of Grümm's theorem), step 1 and the continuity of

$$2(E^{kin} + E^{ext})[\rho(t)] = |||\sqrt{-\Delta}\rho(t)\sqrt{-\Delta}|||_1 + |||\ |x|\rho(t)|x|\ |||_1$$

(cf. lemma 4.3) imply

$$\lim_{t\to s} |||\sqrt{-\Delta}\ (\rho(t)-\rho(s))\sqrt{-\Delta}|||_1 + |||\ |x|\,(\rho(t)-\rho(s))\,|x|\ |||_1 = 0, \quad \forall s \ge 0.$$

Thus

$$\left(\sqrt{-\Delta}\rho(t)\sqrt{-\Delta} + |x|\rho(t)|x|\right) \in C([0,\infty), \tilde{\mathcal{J}}_1(L^2(\mathbb{R}^d)))$$

and the proposition is proved. The case $V_1 \ne 0$ can now be included by a standard perturbation result, *cf.* [Pa] under the additional assumption that $\nabla V_1 \in L^q(\mathbb{R}^d)$, for some $3 \le q \le \infty$, *cf.* [Ar] for the detailed calculations. □

As a remaining preparatory step, the following lemma states an important property of the nonlinear mean field potential $\phi[\rho]$.

Lemma 4.5. *Let $\rho \in \mathcal{E}$ and $d = 3$, then $\phi[\rho] \in L^\infty(\mathbb{R}^3)$. Moreover, the operator $[\phi[\rho], \rho]$ is a local Lipschitz map from $\mathcal{E}$ into itself.*

Proof. In $d = 3$, we explicitly get from (2.14)

$$\phi[\rho] = -\frac{1}{4\pi|x|} * n[\rho], \quad \nabla\phi[\rho] = \frac{x}{4\pi|x|^3} * n[\rho].$$

Therefore, the Hardy-Littlewood-Sobolev inequality and the generalized Young inequality, *cf.* [ReSi2], imply

$$\phi[\rho] \in L^3_w(\mathbb{R}^3) \cap L^p(\mathbb{R}^3), \quad 3 < p < \infty$$

as well as

$$\nabla\phi[\rho] \in L^{3/2}_w(\mathbb{R}^3) \cap L^p(\mathbb{R}^3), \quad 3/2 < p < \infty.$$

Here, L^p_w denotes the weak L^p-spaces, *cf.* [ReSi2]. Hence, by a Sobolev imbedding, $\phi[\rho] \in L^\infty(\mathbb{R}^3)$. Using these estimates, lemma 3.11 of [Ar] shows that $[\phi[\rho], \rho]$ is a local Lipshitz map in the kinetic energy space

$$\mathcal{E}^{kin} := \{\rho \in \tilde{\mathcal{J}}_1 : \sqrt{-\Delta}\rho\sqrt{-\Delta} \in \mathcal{J}_1\} \supset \mathcal{E}. \tag{4.19}$$

Since both, the potential $\phi[\rho]$ and the weight $|x|$ in the functional $E^{ext}[\rho]$ act as multiplication operators, they commute and the local Lipshitz continuity in $\mathcal{E}$ follows. □

We remark that the nonlinear map $\rho \mapsto [\phi[\rho], \rho]$ is continuous in $\mathcal{E}$, but *not* in $\tilde{\mathcal{J}}_1(L^2(\mathbb{R}^3))$ and this is the reason why we need to work in the energy space $\mathcal{E}$. However, the linear evolution problem (3.1) in general does *not* generate a *contractive* QDS on $\mathcal{E} \subset \mathcal{J}_1$, except in the case of a unitary dynamic (*i.e.* $L_j = 0$). Hence, in order to obtain a global-in-time (nonlinear) existence and uniqueness result, we can not apply the results of [AlMe], which would require contractivity of the linear QDS in $\mathcal{E}$.
In the nonlinear evolution problem (4.1) the situation is even worse. Already in the case of a unitary time-evolution only $E^{tot}[\rho(t)]$ is conserved (for $\mu = 0$), whereas $\|\rho(t)\|_{\mathcal{E}}$ is not, due to the possible energy exchange between the potential and the kinetic parts. Hence a unitary but self-consistent evolution problem does not generate a contractive semigroup in $\mathcal{E}$ either.

With the above results, we are able to state the following local-in-time result:

Theorem 4.6. *Let $\rho_0 \in \mathcal{E}$, $d = 3$ and $V_1 \in L^\infty(\mathbb{R}^3)$ s.t. $\nabla V_1 \in L^q(\mathbb{R}^3)$, for some $3 \le q \le \infty$, then:*

(a) *Locally in time, the nonlinear evolution problem (4.1) has a unique mild solution $\tilde{\Phi}_t(\rho_0) \in C([0,T),\mathcal{E})$, where $\tilde{\Phi}_t(\cdot)$ denotes the nonlinear semigroup obtained by perturbing the linear QDS with the Hartree potential. This self-consistent potential satisfies: $\phi \in C([0,T);C_b(\mathbb{R}^3))$. The map $\rho_0 \mapsto \tilde{\Phi}_t(\rho_0)$ is Lipschitz continuous on some (small enough) ball $\{\|\rho - \rho_0\|_{\mathcal{E}} < \varepsilon\} \subset \mathcal{E}$, uniformly for $0 \le t \le T_1 < T$. Further, if the maximum time of existence $T > 0$ is finite, we have*

$$\lim_{t \nearrow T} \|\tilde{\Phi}_t(\rho_0)\|_{\mathcal{E}} = \infty. \tag{4.20}$$

(b) *For $\mathcal{L}(\rho_0) \in \mathcal{E}$ we obtain a classical solution $\tilde{\Phi}_t(\rho_0) \in C^1([0,T),\mathcal{E})$.*
(c) *The semigroup $\tilde{\Phi}_t$ is conservative.*
(d) *The semigroup $\tilde{\Phi}_t$ is positivity preserving and contractive on $\tilde{\mathcal{J}}_1(L^2(\mathbb{R}^3))$. Hence, it furnishes a nonlinear QDS: $\tilde{\Phi}_t : \mathcal{E} \to \mathcal{E} \subset \tilde{\mathcal{J}}_1$.*

Proof. Part (a, b): By proposition 4.4 the unique conservative QDS Φ_t, obtained from theorem 3.9, also maps the energy space $\mathcal{E}$ into itself. Lemma 4.5 and a standard perturbation result (*cf.* theorem 6.1.4 in [Pa]) then yield the local-in-time existence of a solution for the nonlinear, *i.e.* mean field problem. The continuity of ϕ follows from the proof of lemma 4.5, using $\tilde{\Phi}_t(\rho_0) \in C([0,T);\mathcal{E})$. The local Lipschitz continuity of the map $\rho_0 \mapsto \tilde{\Phi}_t(\rho_0)$ follows from theorem 6.1.2 in [Pa] and the uniform lower bound for the existence time of trajectories $\tilde{\Phi}_t(\rho)$ that start in the neighborhood of ρ_0 (cf. proof of theorem 6.1.4 in [Pa]).
Part (c): The proof follows from Duhamel's representation, analogous to (3.26).

Part (d): Having in mind the result of part (a), we consider the nonlinear evolution problem (4.1) as a linear evolution problem with time-dependent Hamiltonian and write it in the following form:

$$\begin{cases} \frac{d}{dt}\rho = -i\,[H,\rho] + A(\rho) - i[\phi(t),\rho], \quad t>0, \\ \rho(0) = \rho_0 \geq 0. \end{cases} \tag{4.21}$$

Here, $\phi \in C([0,T];C_b(\mathbb{R}^3))$ is the self-consistent potential $\phi[\rho]$. To prove the assertions of part (d), we shall approximate $\phi(t)$ on $[0,T_1]$, $T_1 < T$, by the piecewise constant potential:

$$\vartheta(t) := \phi(t_n), \quad t_n \leq t < t_{n+1},\ 0 \leq n \leq N-1,$$

with the uniform grid points: $t_n = n\Delta t$, $\Delta t = T_1/N$. Hence, $\rho(t)$, $t \in [0,T_1]$ is approximated by $\sigma_N \in C([0,T_1];\tilde{\mathcal{J}}_1(L^2(\mathbb{R}^3)))$, solving

$$\begin{cases} \frac{d}{dt}\sigma_N = -i\,[H,\sigma_N] + A(\sigma_N) - i[\vartheta(t),\sigma_N], \quad t>0, \\ \sigma_N(0) = \rho_0 \geq 0. \end{cases} \tag{4.22}$$

Since $\vartheta(t) \in C_b(\mathbb{R}^3)$, corollary 3.10 applies to the generator in (4.22) on each time-intervall $[t_n,t_{n+1}]$. In summary we have the following facts:
ϕ is uniformly continuous on $[0,T_1]$ w.r.t. $\|\cdot\|_\infty$, the solutions of (4.21) satisfies: $|||\rho(t)|||_1 \leq K$, on $0 \leq t \leq T_1$, and the propagator corresponding to (4.22) is contractive on $\tilde{\mathcal{J}}_1(L^2(\mathbb{R}^3))$.
With these ingredients it is standard to verify that

$$\lim_{N\to\infty} \sigma_N = \rho, \quad \text{in } C([0,T_1];\tilde{\mathcal{J}}_1(L^2(\mathbb{R}^3))),$$

cf. the proof of theorem 1 in [AlMe] *e.g.*. Hence, the positivity of $\rho(t) = \tilde{\Phi}_t(\rho_0)$ follows from the positivity of $\sigma_N(t)$.
Analogously, the contractivity of the propagator corresponding to (4.22) implies the contractivity of $\tilde{\Phi}_t(\rho_0)$ in $\tilde{\mathcal{J}}_1(L^2(\mathbb{R}^3))$. □

Remark 4.7. If no confinement potential is present and $\mathrm{Im}(\alpha_{j,k}\overline{\alpha}_{j,l}) = 0$, $\forall j,k,l$, then theorem 4.6 also holds in the kinetic energy space $\mathcal{E}^{kin}$. In particular, this is true for the QFP equation, where one can derive an exact ODE for the kinetic energy, *cf.* [ALMS].

In the next section we shall derive a-priori estimates on $\tilde{\Phi}_t(\rho)$ to prove the global-in-time existence of a conservative QDS for the mean field problem.

5 A-priori estimates and global existence of the mean field QDS

From theorem 4.6, we already know that $|||\rho(t)|||_1 = |||\rho_0|||_1$, for $0 \leq t < T$. It remains to prove an a-priori estimate on the energy of the nonlinear system. As a preliminary step, we introduce a generalized version of the *Lieb-Thirring inequality*:

Lemma 5.1. *Assume $d = 3$ and let $\rho \in \tilde{\mathcal{J}}_1$, $\rho \geq 0$ be s.t. $E^{kin}[\rho] < \infty$. Then the following estimate holds:*

$$\|n[\rho]\|_p \leq K_p \, |||\rho|||_1^\theta E^{kin}[\rho]^{1-\theta}, \quad 1 \leq p \leq 3, \tag{5.1}$$

with

$$\theta := \frac{3-p}{2p}. \tag{5.2}$$

Proof. The proof is given in the appendix of [Ar], *cf.* also [LiPa]. □

In the sequel this estimate will be used to derive an a-priori bound for the total energy.

Proposition 5.2. *Assume $\rho_0 \in \mathcal{E}$, $\rho_0 \geq 0$ and $d = 3$. Then there exists a $K > 0$ such that*

$$E^{tot}[\rho(t)] \leq e^{Kt} E^{tot}[\rho_0], \quad 0 \leq t < T, \tag{5.3}$$

where $\rho(t) := \tilde{\Phi}_t(\rho_0)$, denotes the unique local-in-time solution of the nonlinear evolution problem (4.1).

Proof. Since $\tilde{\Phi}_t$ is positivity preserving, we assume w.r.o.g. $\rho_0 \geq 0$ and hence have $\rho(t) \geq 0$, for all $0 \leq t < T$. The idea is again to derive a differential inequality for E^{tot}. We first consider a classical solution $\tilde{\Phi}_t(\rho_0) \in C^1([0,T), \mathcal{E})$ obtained from an initial condition with $\mathcal{L}(\rho_0) \in \mathcal{E}$.

Step 1: We calculate the time derivative of the total energy, using the short notation $\dot{\rho} \equiv \frac{d}{dt}\rho$:

$$\begin{aligned}\frac{d}{dt} E^{tot}[\rho] &= \frac{d}{dt} \operatorname{Tr}\left(-\frac{1}{2}|\nabla|\rho|\nabla| + \frac{1}{2}|x|\rho|x| + \phi[\rho]\rho\right) - \frac{1}{2}\frac{d}{dt}\operatorname{Tr}(\phi[\rho]\rho) \\ &= \operatorname{Tr}\left(-\frac{1}{2}|\nabla|\dot{\rho}|\nabla| + \frac{1}{2}|x|\dot{\rho}|x| + \phi[\rho]\dot{\rho}\right) + \operatorname{Tr}(\dot{\phi}[\rho]\rho) \\ &\quad - \frac{1}{2}\frac{d}{dt}\operatorname{Tr}(\phi[\rho]\rho).\end{aligned} \tag{5.4}$$

For our classical solution $\rho(t)$ the calculation (5.4) is rigorous since $\|\rho\|_{\mathcal{E}} \in C^1[0,T)$ and the self-consistent potential satisfies $\Phi \in C^1([0,T); C_b(\mathbb{R}^3))$.

In order to simplify the last term on the r.h.s. of (5.4) we evaluate the trace in the eigenbasis of ρ (cf. (2.6)). This gives

$$\frac{1}{2}\frac{d}{dt}\operatorname{Tr}(\phi[\rho]\rho) = \frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^3} \phi(x) n(x) dx.$$

We now proceed as in [Ar]: Integrating by parts several times and using the Poisson equation (2.13), we obtain

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\operatorname{Tr}(\phi[\rho]\rho) &= \frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^3} |\nabla\phi[\rho](x)|^2 dx = -\int_{\mathbb{R}^3} \dot{\phi}[\rho](x)\Delta\phi[\rho](x) dx \\ &= \int_{\mathbb{R}^3} \dot{\phi}[\rho](x) n[\rho](x) dx = \operatorname{Tr}(\dot{\phi}[\rho]\rho).\end{aligned}$$

Inserting this into (5.4), we get

$$\begin{aligned}\frac{d}{dt}E^{tot}[\rho] &= \operatorname{Tr}\left(-\frac{1}{2}|\nabla|\dot{\rho}|\nabla| + \frac{1}{2}|x|\dot{\rho}|x| + \phi[\rho]\dot{\rho}\right)\\ &= \operatorname{Tr}\left(-\frac{1}{2}|\nabla|\mathcal{L}(\rho)|\nabla| + \frac{1}{2}|x|\mathcal{L}(\rho)|x| + \phi[\rho]\mathcal{L}(\rho)\right). \qquad (5.5)\end{aligned}$$

In the following, we shall derive a differential inequality for $E^{tot}[\rho]$ from (5.5). This expression is now considerable easier to deal with, since the self-consistent potential enters as if it was an additional external field (note that the factor $1/2$ in front of $\phi[\rho]$ has been eliminated).

Step 2: Similarly to the proof of lemma 4.3, we introduce an energy-functional

$$E_{k,l}^{tot}[\rho] := E_{k,l}^{kin}[\rho] + E_{k,l}^{ext}[\rho] + \frac{1}{3}E^{sc}[\rho], \quad k,l = 1,2,3,$$

where $E_{k,l}^{kin}$, $E_{k,l}^{ext}$ are defined as in (4.12). Again, for all $\rho \in \mathcal{D}_\infty$, we have

$$E^{tot}[\rho] = \sum_{k=1}^{3} E_{k,k}^{tot}[\rho]$$

and, by a density argument, this carries over to $\rho \in \mathcal{E}$. After some lengthy, but straightforward calculations (with extensive use of the cyclicity of the trace), we get from (5.5), the following equation:

$$\begin{aligned}\frac{d}{dt}\sum_{k=1}^{3} E_{k,k}^{tot} = &\left(\frac{d}{dt}\sum_{k=1}^{3} E_{k,k}^{kin} - \frac{i}{2}\sum_{k=1}^{3}\sum_{j=1}^{M}\operatorname{Tr}((\partial_k^2\phi[\rho])\rho + (\partial_k\phi[\rho])(\partial_k\rho))\right)\\ &+ \frac{d}{dt}\sum_{k=1}^{3} E_{k,k}^{ext} + 2i\mu\sum_{k=1}^{3}\operatorname{Tr}(x_k\rho\partial_k\phi[\rho])\\ &- i\sum_{k,l=1}^{3}\sum_{j=1}^{M}\operatorname{Im}(\overline{\alpha_{j,k}}\beta_{j,l})\operatorname{Tr}(x_k\rho\partial_l\phi[\rho])\\ &- i\sum_{k=1}^{3}\sum_{j=1}^{M}\operatorname{Im}(\overline{\gamma_j}\beta_{j,k})\operatorname{Tr}(\rho\partial_k\phi[\rho]). \qquad (5.6)\end{aligned}$$

Note that the first term of the r.h.s. of (5.6) – in big brackets – equals the time derivative of $E_{k,k}^{kin}$ under the *linear* time-evolution. It is given by (4.14). On the other hand, one easily checks that the time derivative of $E_{k,k}^{ext}$ under the nonlinear time-evolution is equal to the linear one, hence given by (4.15). Since these kinetic and the external (potential) energy terms can be treated (by interpolation arguments) as in the proof of lemma 4.3, it remains to estimate the last three terms on the r.h.s. of (5.6).

Keep in mind, that we want to use a Gronwall lemma in the end. Hence, we need to find appropriate *linear* bounds for the r.h.s. of (5.6). (In the following we shall denote by K positive, not necessarily equal, constants.)

Step 3: We first consider the term $\operatorname{Tr}(\rho\partial_k\phi[\rho])$:

In order to calculate the trace, we need to guarantee that $\rho\partial_k\phi[\rho] \in \mathcal{J}_1$. Using the Sobolev inequality we estimate for $\varphi \in L^2(\mathbb{R}^3)$:

$$\|(|\nabla| + I)^{-1}\varphi\|_6 \leq K\,\|(|\nabla| + I)^{-1}\varphi\|_{H^1} \leq K\,\|\varphi\|_2,$$

since $\|(|\nabla| + I) \cdot \|_2$ is an equivalent norm to $\| \cdot \|_{H^1}$. Hölder's inequality and the bounds obtained in the proof of lemma (4.5) then imply

$$\begin{aligned} \|(\partial_k \phi[\rho])(|\nabla| + I)^{-1} \varphi\|_2 &\leq \|\partial_k \phi[\rho]\|_3 \; \|(|\nabla| + I)^{-1} \varphi\|_6 \\ &\leq K \|\partial_k \phi[\rho]\|_3 \; \|\varphi\|_2 . \end{aligned}$$

In other words, $(\partial_k \phi[\rho])(|\nabla| + I)^{-1}$ is a bounded operator on $L^2(\mathbb{R}^3)$ and we get

$$\begin{aligned} \|| \rho \partial_k \phi[\rho] \||_1 &\leq \||\, (\partial_k \phi[\rho])(|\nabla| + I)^{-1} \||_\infty \; \||\, (|\nabla| + I) \rho \, \||_1 \\ &\leq K \|\partial_k \phi[\rho]\|_3 \, (E^{kin}[\rho] + \||\rho\||_1). \end{aligned}$$

Thus $\rho \partial_k \phi[\rho] \in \mathcal{J}_1$, so we can calculate its trace in the eigenbasis of ρ and estimate it:

$$|\operatorname{Tr}(\rho \partial_k \phi[\rho])| = \left| \int_{\mathbb{R}^3} \partial_k \phi[\rho](x) n[\rho](x) dx \right| \leq \|\nabla \phi[\rho]\|_2 \; \|n[\rho]\|_2 .$$

The generalized Young inequality and the Lieb-Thirring inequality (5.1) imply

$$\|\nabla \phi[\rho]\|_2 \leq K \|n[\rho]\|_{6/5} \leq K \||\rho\||_1^{3/4} E^{kin}[\rho]^{1/4}. \tag{5.7}$$

Further, using again (5.1), we have

$$\|n[\rho]\|_2 \leq K \||\rho\||_1^{1/4} E^{kin}[\rho]^{3/4}.$$

Hence, we obtain the following estimate:

$$|\operatorname{Tr}(\rho \partial_k \phi)| \leq K \||\rho\||_1 \; E^{kin}[\rho], \tag{5.8}$$

which is suitable for our purpose, due to the linear dependence on $E^{kin}[\rho]$.

Step 4: Next, we need to estimate the term

$$\sum_{k,l=1}^{3} \xi_{k,l} \operatorname{Tr}(x_k \rho \partial_l \phi[\rho]),$$

with the short-hand $\xi_{k,l} := \operatorname{Im}(\overline{\alpha_{j,k}} \beta_{j,l})$.

To guarantee that $x_k \rho \partial_l \phi[\rho] \in \mathcal{J}_1$, we only need to show $\sqrt{\rho} \partial_l \phi[\rho] \in \mathcal{J}_2$, since we already know $x_k \sqrt{\rho} \in \mathcal{J}_2$. This can be done as in step 3 above by noting that $\sqrt{\rho}(|\nabla| + I) \in \mathcal{J}_2$ and $(|\nabla| + I)^{-1} \partial_l \phi[\rho] \in \mathcal{B}(L^2(\mathbb{R}^3))$.

Hence, we can again calculate $\operatorname{Tr}(x_k \rho \partial_l \phi[\rho])$ in the eigenbasis of ρ:

$$\begin{aligned} \sum_{k,l=1}^{3} \xi_{k,l} \operatorname{Tr}(x_k \, \rho \, \partial_l \phi[\rho]) &= \sum_{k,l=1}^{3} \xi_{k,l} \int_{\mathbb{R}^3} x_k \, \partial_l \phi[\rho](x) \, n[\rho](x) dx \\ &= - \sum_{k,l,m=1}^{3} \xi_{k,l} \int_{\mathbb{R}^3} x_k \, \partial_l \phi[\rho](x) \, \partial^2_{m,m} \phi[\rho](x) dx, \end{aligned} \tag{5.9}$$

where we have used the Poisson equation (2.13) for the last equality. Integration by parts gives

$$\begin{aligned} \sum_{k,l=1}^{3} \xi_{k,l} \operatorname{Tr}(x_k \, \rho \, \partial_l \phi[\rho]) = &\sum_{k,l=1}^{3} \xi_{k,l} \int_{\mathbb{R}^3} \partial_l \phi[\rho](x) \, \partial_k \phi[\rho](x) dx \\ &+ \sum_{k,l,m=1}^{3} \xi_{k,l} \int_{\mathbb{R}^3} x_k \partial^2_{l,m} \phi[\rho](x) \, \partial_m \phi[\rho](x) dx. \end{aligned} \tag{5.10}$$

Adding the equations (5.10) and (5.9) yields, after another integration by parts:

$$
\begin{aligned}
&2 \sum_{k,l=1}^{3} \xi_{k,l} \operatorname{Tr}(x_k\, \rho\, \partial_l \phi[\rho]) \\
&= \sum_{k,l=1}^{3} \xi_{k,l} \int_{\mathbb{R}^3} \partial_l \phi\, \partial_k \phi\, dx \sum_{k,l,m=1}^{3} \xi_{k,l} \int_{\mathbb{R}^3} \left[x_k\, \partial_m \phi\, \partial^2_{l,m} \phi - x_k\, \partial_l \phi\, \partial^2_{m,m} \phi\right] dx \\
&= \sum_{k,l=1}^{3} \xi_{k,l} \int_{\mathbb{R}^3} \partial_l \phi\, \partial_k \phi\, dx \\
&\quad - \sum_{k,l,m=1}^{3} \xi_{k,l} \int_{\mathbb{R}^3} \left[\delta_{k,m}\, \partial^2_{l,m} \phi + x_k\, \partial^3_{l,m,m} \phi - \delta_{k,l}\, \partial^2_{m,m} \phi - x_k\, \partial^3_{l,m,m} \phi\right] \phi\, dx \\
&= 2 \sum_{k,l=1}^{3} \xi_{k,l} \int_{\mathbb{R}^3} \partial_l \phi\, \partial_k \phi\, dx - \sum_{k,m=1}^{3} \xi_{k,k} \int_{\mathbb{R}^3} |\partial_m \phi|^2\, dx, \qquad (5.11)
\end{aligned}
$$

where we write $\phi \equiv \phi[\rho]$ for simplicity and denote by $\delta_{k,l}$ the Kronecker symbol. Therefore we can estimate

$$
\left| \sum_{k,l=1}^{3} \xi_{k,l} \operatorname{Tr}(x_k \rho \partial_l \phi[\rho]) \right| \le K\, \|\nabla \phi[\rho]\|_2^2,
$$

where K depends on the coefficients $\xi_{k,l}$.
Hence, using the same estimates as in (5.7), we have

$$
\begin{aligned}
\left| \sum_{k,l=1}^{3} \xi_{k,l} \operatorname{Tr}(x_k \rho \partial_l \phi[\rho]) \right| &\le K\, |||\rho|||_1^{3/2}\; E^{kin}[\rho]^{1/2} \\
&\le K\, |||\rho|||_1 \left(|||\rho|||_1 + E^{kin}[\rho]\right),
\end{aligned}
$$

which is the desired linear bound.
The third term in (5.6) can be treated analogously to the previous case.
Step 5: The steps 1-4, together with the estimates obtained in the proof of lemma 4.3, imply

$$
\frac{d}{dt} E^{tot}[\rho(t)] \le\; K E^{tot}[\rho(t)], \quad 0 \le t < T, \qquad (5.12)
$$

with some generic constant $K \ge 0$. Applying Gronwall's lemma then proves the assertion.

Strictly speaking, all the calculations of steps $2-5$ first have to be done for an approximating sequence $\{\sigma_n\} \subseteq \mathcal{D}_\infty$, such that $\sigma_n \overset{n\to\infty}{\longrightarrow} \rho(t)$ in $\mathcal{E}$ for each fixed $t \in [0,T)$ (*cf.* the proof of theorem 3.9). The estimate (5.12) then also holds for the limit $\rho(t)$ since the constant K is independent of $\{\sigma_n\}$.

Step 6: So far we have proved (5.3) for classical solutions. By theorem 4.6(a) any mild solution (i.e. $\tilde{\Phi}_t(\rho_0) \in C([0,T),\mathcal{E})$) can be approximated in $\mathcal{E}$ (uniformly on $0 \le t \le T_1 < T$) by classical solutions. Hence (5.3) carries over to all initial conditions $\rho_0 \in \mathcal{E}$ with $\rho_0 \ge 0$. □

In view of (4.20), and since $\|\rho(t)\|_{\mathcal{E}} \le E^{tot}[\rho(t)]$ we conclude from the above proposition that $T = \infty$ and obtain our main result:

Theorem 5.3. *Let $\rho_0 \in \mathcal{E}$, $d = 3$ and $V_1 \in L^\infty(\mathbb{R}^3)$ s.t. $\nabla V_1 \in L^q(\mathbb{R}^3)$, for some $3 \le q \le \infty$:*

Then, the nonlinear evolution problem (4.1) admits a unique mild solution, i.e. it generates a nonlinear conservative QDS: $\tilde{\Phi}_t(\rho_0) \in C([0,\infty), \mathcal{E})$.

6 Appendix: Proof of Lemma 3.7

Without loss of generality we can assume that ρ is a nonnegative operator. (Otherwise one can split ρ into its positive and negative part [ReSi1] and prove the result separately for each one.) Its eigenvalues are $\lambda_j \ge 0$ and the eigenvectors ψ_j are orthonormal.

Part (a): For each $\rho \in \tilde{\mathcal{J}}_1$ and the corresponding sequence $\{\sigma_n\} \subset \mathcal{D}_\infty$, defined in (3.17), we need to show that

$$\lim_{n\to\infty} |||\rho - \sigma_n|||_1 = 0.$$

Note that it is enough to prove the result for $\rho \in \tilde{\mathcal{J}}_1$ with finite rank $N \in \mathbb{N}$, since finite rank operators are dense in $\tilde{\mathcal{J}}_1$, *cf.* [ReSi1]. With the kernel of $\sigma_n \in \tilde{\mathcal{J}}_1$ as in (3.18), we get from (3.13), that for all $f \in L^2(\mathbb{R}^d)$

$$\lim_{n\to\infty} (\sigma_n f)(x) = \lim_{n\to\infty} \sum_{j=1}^{N} \lambda_j \; \varphi_{j,n}(x) \int_{\mathbb{R}^d} \overline{\varphi_{j,n}(y)} \; f(y)dy = (\rho f)(x)$$

in $L^2(\mathbb{R}^d)$, *i.e.* the operators $\sigma_n \to \rho$ in the strong operator topology. Since we assumed that ρ has finite rank, we conclude from (3.19) that the trace norms converge, *i.e.*

$$\lim_{n\to\infty} |||\sigma_n|||_1 = |||\rho|||_1.$$

Combining these two results, the theorem of Grümm (theorem 2.19 of [Si]) implies that $\sigma_n \to \rho$ in $\mathcal{J}_1$.

Part (b): The inclusion $\mathcal{D}(Z) \subset \mathcal{D}(\mathcal{L})$ is already clear from proposition 3.6. Thus it remains to show that for each $\sigma_n \in \mathcal{D}_n \subset \mathcal{D}_\infty$, with some fixed $n \in \mathbb{N}$, we have $Z(\sigma_n) \in \tilde{\mathcal{J}}_1$:

First note that $Z(\sigma_n) := Y\sigma_n + \sigma_n Y^*$ is a linear combination of the following terms (and their adjoints)

$$x_k\sigma_n x_l,\ \partial_k\sigma_n\partial_l,\ \partial_k\sigma_n x_l,\ x_k x_l\sigma_n,\ \partial_k\partial_l\sigma_n,\ x_k\partial_l\sigma_n,\ x_k\sigma_n,\ \partial_k\sigma_n, \qquad \text{(A.1)}$$

where $1 \le k,l \le d$ and $\partial_k := \partial_{x_k}$. (Indeed not all of this terms really appear in the expression of Z, but since the same argument for $\mathcal{L}$ is needed in the proof of theorem 3.9, we shall consider this more general case.)

Since σ_n has a representation given by $\sigma_n = M(\chi_n)C(\varphi_n)\rho\; C(\varphi_n)M(\chi_n)$, for some $\rho \in \tilde{\mathcal{J}}_1$, we have to prove that the operator compositions $x^a\nabla^b M_n C_n$ are in $\mathcal{B}(L^2(\mathbb{R}^d))$. Here the multi-indices $a, b \in \mathbb{N}_0^d$ are such that $|a| + |b| \le 2$. As an example we consider the operator $x_k\partial_l$ and write for $f \in L^2(\mathbb{R}^d)$:

$$\begin{aligned}(x_k\partial_l M_n C_n f)(x) &= x_k\partial_l(\chi_n(x)(\varphi_n * f)(x)) \\ &= x_k[\partial_l\chi_n(x)(\varphi_n * f)(x) + \chi_n(x)(\partial_l\varphi_n * f)(x)].\end{aligned}$$

Since $\varphi, \chi \in C_0^\infty$ (see the proof of lemma 3.3) we have that

$$\|x_k \partial_l M_n C_n f\|_2 \leq K_{k,l,n} \|f\|_2$$

and hence $x_k \partial_l M_n C_n \in \mathcal{B}(L^2(\mathbb{R}^d))$. Therefore $x_k \partial_l \sigma_n = x_k \partial_l M_n C_n \rho C_n M_n \in \tilde{\mathcal{J}}_1$. The other terms in (A.1) can then be handled in a similar way.

Part (c): After the proof of part (a) it remains to show that for all $\rho \in \tilde{\mathcal{J}}_1$ with $\mathcal{L}(\rho) \in \tilde{\mathcal{J}}_1$, the following statement holds:

$$\lim_{n\to\infty} |||\mathcal{L}(\sigma_n) - \mathcal{L}(\rho)|||_1 = 0.$$

To simplify the proof, it is sufficient to consider a "model operator" $\mathcal{K}(\rho)$, for which we choose $l = k = 1$ in (A.1) and further set all constants equal to one. This simplification is possible since no cancellation occurs between the individual terms of $\mathcal{K}(\rho)$. To simplify the notation further, we shall from now on write $v := x_1$, $\partial := \partial_{x_1}$. We choose $\mathcal{K}$ in the form

$$\mathcal{K}(\rho) = \mathcal{K}_1(\rho) + \mathcal{K}_1(\rho)^*,$$

where

$$\mathcal{K}_1(\rho) = v\rho v + \partial\rho\partial + \partial\rho v + v^2\rho + \partial^2\rho + v\partial\rho + v\rho + \partial\rho.$$

The general (d - dimensional) case $\mathcal{L}(\rho) = -i[H,\rho] + A(\rho)$ described above is then a straightforward extension. The proof now follows again in several steps:

Step 1: We write

$$\begin{aligned}\mathcal{K}(\sigma_n) &\equiv \mathcal{K}\big(M(\chi_n)C(\varphi_n)\rho\ C(\varphi_n)M(\chi_n)\big)\\ &= M(\chi_n)C(\varphi_n)\mathcal{K}(\rho)\ C(\varphi_n)M(\chi_n) + R_n(\rho) + R_n(\rho)^*.\end{aligned}$$

Since $\mathcal{K}(\rho) \in \tilde{\mathcal{J}}_1$, we can decompose it, *cf.* [ReSi1] into

$$\mathcal{K}(\rho) = \mathcal{K}_+(\rho) - \mathcal{K}_-(\rho),$$

with $\mathcal{K}_\pm(\rho) \geq 0$. Applying part (a) of this lemma then yields

$$\lim_{n\to\infty} |||\ M(\chi_n)C(\varphi_n)\mathcal{K}(\rho)\ M(\chi_n)C(\varphi_n) - \mathcal{K}(\rho)\ |||_1 = 0.$$

It remains to prove that $R_n(\rho) \to 0$ in $\mathcal{J}_1$, as $n \to \infty$, which also implies $R_n(\rho)^* \to 0$ in $\mathcal{J}_1$. For technical reasons (which will become clear in step 3) we split this remainder term into two parts: $R_n(\rho) = R_n^1(\rho) + R_n^2(\rho)$, and treat each of them separately.

Step 2: After some lengthy calculations, $R_n^1(\rho)$ can be written as

$$\begin{aligned}R_n^1(\rho) = {} & M(\partial\chi_n)C(\varphi_n)\,\rho\, C(\varphi_n)M(\partial\chi_n)\\ & + M(\partial^2\chi_n)C(\varphi_n)\,\rho\, C(\varphi_n)M(\chi_n)\\ & + M(\chi_n)C(v\varphi_n)\rho\, C(\varphi_n)M(\chi_n)\\ & + M(\partial\chi_n)C(\varphi_n)\,\rho\, C(\varphi_n)M(\chi_n)\\ & - M(\chi_n)C(v^2\varphi_n)\,\rho\, C(\varphi_n)M(\chi_n)\\ & - 2\, M(\chi_n)C(v\varphi_n)\,\rho\, C(v\varphi_n)M(\chi_n),\end{aligned}$$

where, on the level of the kernels, we have used several times the basic identity

$$v(f * g) = vf * g + f * vg.$$

Now we calculate for $f \in L^2(\mathbb{R}^d)$ (remember $v = x_1$)

$$\begin{aligned}(C(x_1\varphi_n)f)(x) &:= \int_{\mathbb{R}^d} (x_1 - y_1)\ \varphi_n(x-y) f(y) dy \\ &= \frac{1}{n}\int_{\mathbb{R}^d} n^{d+1}(x_1 - y_1)\ \varphi(n(x-y)) f(y) dy = O\left(n^{-1}\right).\end{aligned}$$

Thus we have for the operator norm $|||C(v\varphi_n)|||_\infty = O\left(n^{-1}\right)$. Similarly we obtain

$$\begin{aligned}&|||C(\varphi_n)|||_\infty = |||M(\chi_n)|||_\infty = O(1),\\ &|||M(\partial\chi_n)|||_\infty = O\left(n^{-1}\right),\\ &|||C(v^2\varphi_n)|||_\infty = |||M(\partial^2\chi_n)|||_\infty = O\left(n^{-2}\right).\end{aligned}$$

With these relations we can estimate, using $|||AB|||_1 \leq |||A|||_\infty\,|||B|||_1$, *cf.* [ReSi1]

$$\begin{aligned}|||\ R_n^1(\rho)\ |||_1 \leq\ & |||\rho|||_1\ |||M(\chi_n)|||_\infty^2 |||C(v\varphi_n)|||_\infty^2 \\ &+\ |||\rho|||_1\ |||M(\chi_n)|||_\infty^2 |||C(\varphi_n)|||_\infty\ |||C(v^2\varphi_n)|||_\infty \\ &+\ |||\rho|||_1\ |||C(\varphi_n)|||_\infty^2 |||M(\partial\chi_n)|||_\infty^2 \\ &+\ |||\rho|||_1\ |||C(\varphi_n)|||_\infty^2 |||M(\chi_n)|||_\infty\ \|M(\partial^2\chi_n)\|_\infty \\ &+\ |||\rho|||_1 |||C(\varphi_n)|||_\infty |||M(\chi_n)|||_\infty^2 |||C(v\varphi_n)|||_\infty \\ &+\ |||\rho|||_1 |||C(\varphi_n)|||_\infty^2 |||M(\chi_n)|||_\infty\ |||M(\partial\chi_n)|||_\infty \\ =\ & O\left(n^{-1}\right).\end{aligned}$$

Thus $R_n^1(\rho) \to 0$ uniformly in $\mathcal{J}_1$, as $n \to \infty$.

Step 3: Again a lengthy, but straightforward calculation shows that the second part of the remainder can be written in the form

$$\begin{aligned}R_n^2(\rho) =\ & M(n\partial\chi_n)C(\varphi_n)\,\rho\,C(\frac{\partial\varphi_n}{n})M(\chi_n) \\ &+\ M(\chi_n)C(\partial(v\varphi_n))\,\rho\,C(\varphi_n)M(\chi_n) \\ &+\ M(\chi_n)C(\frac{\partial\varphi_n}{n})\,\rho\,C(\varphi_n)M(n\partial\chi_n) \\ &+\ M(n\partial\chi_n)C(\varphi_n)\,\rho\,C(\varphi_n)M(\frac{v}{n}\chi_n) \\ &+\ M(\chi_n)C(\frac{\partial\varphi_n}{n})\,\rho\,C(nv\varphi_n)M(\chi_n) \\ &+\ M(v\partial\chi_n)C(\varphi_n)\,\rho\,C(\varphi_n)M(\chi_n) \\ &+\ 2\,M(n\partial\chi_n)C(\frac{\partial\varphi_n}{n})\,\rho C(\varphi_n)M(\chi_n) \\ &+\ M(\frac{v}{n}\chi_n)C(\varphi_n)\,\rho\,C(nv\varphi_n)M(\chi_n) \\ &+\ M(\chi_n)C(nv\varphi_n)\,\rho\,C(\varphi_n)M(\frac{v}{n}\chi_n) \\ &+\ 2\,M(\frac{v}{n}\chi_n)C(nv\varphi_n)\,\rho\,C(\varphi_n)M(\chi_n).\end{aligned}$$

In contrast to step 2 these terms do not converge to zero uniformly in $\mathcal{J}_1$. Therefore we need to proceed differently:
As an example we consider the ninth term on the right hand side and write

$$M(\chi_n)C(nv\varphi_n)\rho\, C(\varphi_n)M(\frac{v}{n}\chi_n) = M(\chi_n)C(nv\varphi_n)\rho^N C(\varphi_n)M(\frac{v}{n}\chi_n) + M(\chi_n)C(nv\varphi_n)(\rho-\rho^N)C(\varphi_n)M(\frac{v}{n}\chi_n),$$

where ρ^N is the trace class operator ρ "cut" at finite rank $N \in \mathbb{N}$, such that $|||\,\rho-\rho^N|||_1 \le \varepsilon$, $\varepsilon \in \mathbb{R}_+$. Direct calculations, similar to the one in step 2, imply

$$|||C(nv\varphi_n)|||_\infty \le K,\ |||M(n^{-1}v\chi_n)|||_\infty \le K,\ K \in \mathbb{R}, \tag{A.2}$$

with K independent of $n \in \mathbb{N}$. Thus we can estimate

$$|||M(\chi_n)\ C(nv\varphi_n)(\rho-\rho^N)\ C(\varphi_n)M(\frac{v}{n}\chi_n)|||_1 \le \varepsilon K^2. \tag{A.3}$$

Define Π to be the projector on $\mathrm{ran}(\rho^N)$. Then $\rho^N = \Pi\rho^N$ and

$$|||C(nv\varphi_n)\rho^N|||_1 \le |||C(nv\varphi_n)\Pi|||_\infty\ |||\rho^N|||_1. \tag{A.4}$$

Now, since $\dim(\mathrm{ran}(\rho^N)) < \infty$ and since strong convergence equals uniform convergence on finite dimensional spaces [ReSi1], we get

$$\lim_{n\to\infty} |||C(nv\varphi_n)\Pi|||_\infty = 0. \tag{A.5}$$

Here we used the fact, that $C(nv\varphi_n)f \to 0$ in $L^2(\mathbb{R}^d)$, for all $f \in L^2(\mathbb{R}^d)$. Combining (A.2) - (A.5) we thus have

$$\lim_{n\to\infty} |||M(\chi_n)\ C(nv\varphi_n)\rho^N\ C(\varphi_n)M(\frac{v}{n}\chi_n)|||_1 = 0. \tag{A.6}$$

Combining (A.3) and (A.6) shows that

$$|||M(\chi_n)\ C(nv\varphi_n)\rho\ C(\varphi_n)M(\frac{v}{n}\chi_n)|||_1$$

can be made arbitrarily small for N sufficiently large. All other terms appearing in the expression of R_n^2 can now be treated in the same way:
The definitions of φ_n and χ_n imply that all the distributions $nv\varphi_n$, $\frac{1}{n}\partial\varphi_n$ and $\partial(v\varphi_n)$ converge to zero in $\mathcal{D}'(\mathbb{R}^d)$. Further we have

$$|n\partial\chi_n| = \left|\chi'\left(\frac{|x|}{n}\right)\frac{v}{|x|}\right| \le K,$$

by assumption. Similarly

$$|v\partial\chi_n| = \left|\frac{v^2}{n|x|}\chi'\left(\frac{|x|}{n}\right)\right|$$

is in $L^\infty(\mathbb{R}^d)$ uniformly for $n \in \mathbb{N}$ with support in the annulus $\frac{n}{2} \le |x| \le n$. Also $\frac{v}{n}\chi_n$ is uniformly in $L^\infty(\mathbb{R}^d)$ with

$$\lim_{n\to\infty} \|n^{-1}v\chi_n\|_{L^\infty(B_R)} = 0$$

on each ball of radius R. Thus we have strong convergence on $\mathrm{ran}(\rho^N)$ for each term of R_n^2.

In summary we have proved in steps 1 to 3 the assertion of the lemma. □

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