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On the Dipole Approximation

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Abstract

The dipole approximation is employed to describe interactions between atoms and radiation. It essentially consists of neglecting the spatial variation of the electromagnetic field over the atom – instead, one uses the field at the location of the nucleus. Heuristically, this procedure is justified by arguing that the wavelength is considerably larger than the atomic length scale, which holds under usual experimental conditions. The aim of this thesis is to make the argument rigorous by proving the dipole approximation in the limit of infinite wavelengths compared to the atomic length scale.

We study the semiclassical Hamiltonians describing the interaction with both the exact and the approximated electromagnetic field and prove existence and uniqueness of the respective time evolution operators. We show that the exact time evolution converges strongly to the approximated operator in said limit.

Based thereupon we identify subspaces of the Hamiltonian's domain which remain invariant under the approximated time evolution. We estimate the rate of convergence for appropriately chosen initial wave functions, and show that it is inversely proportional to the wavelength of the electromagnetic field and besides not uniform in time.

Our results are obtained under physically reasonable assumptions on atomic potential and electromagnetic field. They include N-body Coulomb potentials and experimentally relevant electromagnetic fields such as plane waves and laser pulses.

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Conventions

Throughout this thesis we use the Gaussian unit system. In these units, the Maxwell equations are of the form

$$\begin{aligned}
\nabla \cdot \mathbf{E} &= 4\pi\rho, \\
\nabla \cdot \mathbf{B} &= 0, \\
\nabla \times \mathbf{E} &= -\tfrac{1}{c}\tfrac{\partial \mathbf{B}}{\partial t}, \\
\nabla \times \mathbf{B} &= \tfrac{1}{c}\tfrac{\partial \mathbf{E}}{\partial t} + \tfrac{4\pi}{c}\mathbf{j}.
\end{aligned}$$

Further, we use the Coulomb gauge,

$$\nabla \cdot \mathbf{A} = 0,$$

and put $\hbar \equiv e \equiv 1$ and the electron mass $m \equiv \frac{1}{2}$. In these units, the velocity of light c has a numerical value of about 137.

Elements of $\mathbb{R}^d$ $(d > 1)$ are denoted in **boldface**.

We use the following notation:

- $\mathcal{C}^l(\Omega)$ denotes the set of l times continuously differentiable functions $\mathbb{R}^d \supseteq \Omega \to \mathbb{C}$; the index zero in the case of continuous functions is omitted
- $\mathcal{C}^l_c(\Omega)$ denotes the set of l times continuously differentiable functions $\mathbb{R}^d \supseteq \Omega \to \mathbb{C}$ with compact support
- $\mathcal{H}$ denotes a complex Hilbert space
- $\mathcal{L}(X,Y)$ denotes the set of bounded operators from X into Y; if X and Y are identical, we abbreviate $\mathcal{L}(X,X) \equiv \mathcal{L}(X)$. The operator norm on $\mathcal{L}(X,Y)$ is expressed as $\|\cdot\|_{X\to Y}$; in the case $X = Y$ we write $\|\cdot\|_X$
- $\|x\| \equiv \|x\|_{L^2(\mathbb{R}^d)}$ denotes the $L^2(\mathbb{R}^d)$-norm for elements $x \in L^2(\mathbb{R}^d)$ and $\|A\| \equiv \|A\|_{L^2(\mathbb{R}^d)}$ the respective operator norm for operators A on $L^2(\mathbb{R}^d)$, unless otherwise stated
- $L^p_{\mathrm{loc}}(\Omega) = \left\{ f : \mathbb{R}^d \supseteq \Omega \to \mathbb{C} : f \in L^p(K)\ \forall K \subseteq \Omega \text{ compact } \right\}$
- $\mathcal{S}(\mathbb{R}^d) = \left\{ f \in \mathcal{C}^\infty(\mathbb{R}^d) : \sup\limits_{\mathbf{x}\in\mathbb{R}^d} |\mathbf{x}^\alpha(\partial_\beta f)(\mathbf{x})| < \infty\ \forall \alpha,\beta \in \mathbb{N}_0^n \right\}$ is the Schwartz space

Constants, unless specified, may vary from step to step – even within the same line – and are denoted by C.

1 Introduction

Physics aims at revealing the underlying law describing the world we perceive. For this law to hold universally, we demand that it be written in the language of mathematics and extend to a consistent theory without ambiguities or vague formulations. The ultimate goal is to explain each process in every detail. This aspiration is however extremely ambitious – even for systems with very few particles it is currently often impossible to describe the behaviour *exactly*. Therefore physicists have always employed approximations: better to provide a description capturing the situation approximately than not to gain any insight whatsoever. Considerations of simplified models, permitting to focus on the essential features, have led to the acquisition of much knowledge and understanding.

An approximation widely used by both theoretical and experimental physicists is the *dipole approximation*, sometimes also referred to as the *long wavelength approximation*. It is commonly used for the description of interactions between radiation and atoms.

Let us consider an atom targeted by a laser. Our aim is to describe the interaction between the laser's electromagnetic field and an electron confined within the atom. Typically, the wavelength of the field is considerably greater than the atomic length scale, thus it seems not immoderate to neglect the spatial variation of the electromagnetic field over the atom completely. Said atomic electron sees approximately the same field as the nucleus, which we put in the center of our reference frame. This approximation, i.e. the simplifying assumption that the electromagnetic field is spatially constant on the length scale of the atom, is the dipole approximation. The intention of this thesis is to make the heuristic argument rigorous and to quantify the validity of the approximation.

The central object is the wave function of the electron, whose time evolution is determined via the Schrödinger equation by the interaction Hamiltonian

$$H_\lambda(\mathbf{x}, t) = \Big(\mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{x}, t)\Big)^2 + V(\mathbf{x}),$$

where $V(\mathbf{x})$ denotes the atomic potential. We will justify the specific form of $H_\lambda(t)$ in Chapter 2. For now we merely note that it is a semiclassical Hamiltonian: the electron is treated quantum mechanically whereas the electromagnetic field is described classically by the vector potential $\mathbf{A}(\mathbf{x}, t)$. Applying the dipole approximation essentially means to replace $\mathbf{A}(\mathbf{x}, t)$ by $\mathbf{A}(0, t)$ in the Hamiltonian, resulting in

$$H_\infty(\mathbf{x}, t) = \Big(\mathbf{p} - \frac{e}{c}\mathbf{A}(0, t)\Big)^2 + V(\mathbf{x}).$$

This is equivalent to the above idea of the atomic electron experiencing a spatially constant field. We can expect $H_\infty(t)$ to generate viable results only if the electron is located extremely close to the nucleus on the scale determined by the laser's wavelength λ. We will

confirm that, in this regime, the approximation is indeed good. We prove that the exact time evolution converges strongly to the time evolution in dipole approximation in the limit $\lambda \to \infty$.
The convergence being established, we go one step further and examine its speed. We are particularly interested in gaining some insight regarding two questions: given an initial state of the atom and some time during which it interacts with a laser, which wavelengths may be chosen to guarantee for a good approximation? And conversely, given a laser with a specific wavelength and an atom prepared in a particular way, how long until the approximation ceases to be viable?
We will estimate the rate of convergence for wave functions remaining in some sense localised around the nucleus. The challenge in finding such wave functions is that we are merely able to impose conditions on the *initial* wave function; the behaviour at later times must be deduced from the time evolution. We will therefore prove that the domain of the quantum harmonic oscillator is left invariant by the time evolution, as this space shows just the desired properties: all of its element display a finite kinetic energy, and moreover their variance and the fourth moment in position is finite. This provides sufficient localisation to prove a theorem quantifying the rate of convergence.

Both experimental and theoretical physicists make ample use of the dipole approximation, which can be found in most textbooks treating light-matter interactions. Examples are [1, Ch. 2], [2, Ch. 7] or [3, Ch. 7].
In mathematical physics, the dipole approximation is of particular interest for proofs related to (photo-)ionisation. This phenomenon has been studied from different perspectives: Fröhlich, Pizzo and Schlein [4] make use of the dipole approximation to describe the ionisation of a hydrogen-like atom by a short, very intense laser pulse. Costin, Lebowitz and Stucchio [5] study a one-dimensional model atom interacting with a dipole radiation field $\mathbf{E}(t) \cdot x$,

$$\widetilde{H}(t) = -\Delta + e\mathbf{E}(0,t) \cdot \mathbf{x} + V(\mathbf{x}).$$

As we will see in Chapter 2, the time evolution generated by $\widetilde{H}(t)$ is unitarily equivalent to the one generated by $H_\infty(t)$. In case of a periodically oscillating electric field, this is known as *AC-Stark Effect*, mathematically examined by Graffi and Yajima [6, 7]. A similar Hamiltonian describing two interacting particles in an external time-periodic field is studied by Møller [8]. Pauli and Fierz [9] describe the motion of a charged, spatially extended particle in a force field in the context of non-relativistic QED and use the dipole approximation for the emerging radiation.

To our knowledge, there are only few works justifying the dipole approximation rigorously. Fröhlich, Bach and Sigal [10] consider a system of non-relativistic electrons bound to static nuclei interacting with a quantised electromagnetic field and argue for the use of the dipole approximation in this case. Griesemer and Zenk [11] examine the photo-ionisation of one-electron atoms due to interactions with a quantised radiation field of low intensity. Within the framework of non-relativistic QED, they prove that the ionisation probability is correctly given by formal time-dependent perturbation theory, to leading order in the fine-structure constant α. The authors show that the dipole approximation produces merely an error of sub-leading order, which justifies its validity.
In this thesis, we prove the dipole approximation directly from the time evolution, and

besides include an estimate of the rate of convergence. To achieve this, we make several assumptions on the potential and the electromagnetic field. They are physically reasonable in the sense that Coulomb potentials and laser fields are included.
The motivation for this thesis has been a joint work of Dürr, Grummt and Kolb [12, 13]. The authors prove existence and uniqueness of the time evolution operators, mainly using a theorem from the textbook by Reed and Simon [14, Theorem X.70]. We adopt their general idea as well as some intermediate results, but provide an alternative proof based upon the original and more general theorems of Kato [15] and Yosida [16]. The estimate of the rate of convergence, inspired by works of Radin and Simon [17] and Huang [18], is – to our best knowledge – a new result.

The organisation of this thesis is as follows: we begin Chapter 2 with an outline of the physics involved and define the objects of interest. The mathematical notions and theorems required are introduced in Chapter 3. Chapter 4 is dedicated to the proof of existence and uniqueness of the time evolution operators and the establishment of their strong convergence in the limit of infinite wavelengths. After identifying appropriate subspaces left invariant by the time evolution in Chapter 5, Chapter 6 concludes with an estimate of the rate of convergence for appropriately chosen initial conditions.

2 Dipole Approximation

The dipole approximation is commonly used for the description of the interaction between an electron confined within an atom and an external electromagnetic field. *External* means in this context that the sources of the field are not part of the dynamical system under consideration but remain fixed. The effect on the external sources caused by the field arising from the motion of the electron must therefore be compensated for by the experimental arrangement, or we simply assume that the influence of the electron's field is negligible.
We start from a classical description of the problem and proceed to a semiclassical formulation. Subsequently, we introduce the dipole approximation and show that the approximated Hamiltonian is gauge equivalent to the Hamiltonian describing the coupling of a homogeneous electric field to the electric dipole moment of the electron. By means of this Hamiltonian we describe briefly the phenomenon of ionisation, which provides the main motivation for a proof of the dipole approximation.
The content of this chapter is based on the textbooks of Cohen-Tannoudji *et al.*, in particular [19, Compl. C_{II}, A_{IV} and Ch. IV.B] and [20, Compl. 13.4]. The paragraph concerning ionisation refers to [13, 4].

2.1 Semiclassical Hamiltonian

Let us consider the interaction of a *classical* non-relativistic point particle (electric charge e, mass m) in a potential with a classical external electromagnetic field. We write $\hbar$, e and m in this chapter explicitly (whereas $\hbar = e = 1$ and $m = \frac{1}{2}$ for the rest of the thesis) and besides do not a priori fix the Colomb gauge. We choose our reference frame in such a way that the nucleus of the atom, which is described by the potential $V(\mathbf{x})$, is located at $\mathbf{x} = 0$. The Hamiltonian function describing this interaction reads

$$H(\mathbf{x}, \mathbf{p}, t) = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}_\lambda(\mathbf{x}, t)\right)^2 + e\Phi(\mathbf{x}, t) + V(\mathbf{x}), \tag{2.1}$$

where $\mathbf{A}_\lambda$ denotes the vector potential, Φ the electrostatic potential and V the atomic potential. A derivation through the Lagrange formalism can be found in [21, Ch. 12.1.] and [19, Compl. C_{II}]. A non-relativistic description of the electron seems appropriate, regarding our objective to describe electrons within atoms.
We may choose the Coulomb gauge,

$$\nabla \cdot \mathbf{A}_\lambda = 0,$$

and, as there are no sources of the external field present within the region of interest, obtain $\Phi = 0$. The electric field is consequently determined by

$$\mathbf{E}(\mathbf{x}, t) = -\tfrac{1}{c}\partial_t \mathbf{A}_\lambda(\mathbf{x}, t). \tag{2.2}$$

We go now one step further and describe the interaction *semiclassically*: we treat the electron as a quantum particle whereas describing the electromagnetic field classically. This might seem awkward, as expressed by KEMBLE in his textbook on quantum mechanics:

> *[...] the reader will be inclined to raise his eyebrows at the attempt to combine a quantum theory of the atom with a classical picture of an interacting electromagnetic field. Our excuse for the construction of such a hybrid theory lies partly in the observation that in the limiting case of very long wave lengths – static or quasi-static fields – the corpuscular properties of the electromagnetic field recede into the background while the classical properties dominate. Hence we can reasonably hope that such a classical treatment of the field will be in asymptotic agreement with experiment as the wave lengths under consideration become very large. [22, Ch. 1]*

Treating $\mathbf{A}_\lambda$ as a classical electromagnetic field means that we consider the influence of $\mathbf{A}_\lambda$ on the electron but not vice versa. Whereas $\mathbf{A}_\lambda$ may cause the electron to change its state, $\mathbf{A}_\lambda$ itself is not altered. This seems a reasonable approximation if the intensity of the electromagnetic field is adequately high: it is of no great importance whether one photon more or less is contained in the radiation field, if only the number of photons hitting the atom is sufficiently great. For weak or no incident radiation however, the change in the radiation field may not be neglected as easily [1, Ch. 2.4].
The dipole approximation is used in situations such as lasers interacting with atoms, in particular for the phenomena of ionisation and atomic transitions. In these cases, the high intensity is usually given, and besides we will be concerned about wavelengths much greater than the atomic length scale.
Moreover, there exists so far no completely rigorous quantum mechanical description of photons. Although the semiclassical treatment has its limitations, it is the best we have to offer, and it describes the phenomena observed in laboratories very well.

Following the customary recipe to convert the classical Hamiltonian function (2.1) into an operator, we arrive at the Hamiltonian in position representation

$$H_\lambda(\mathbf{x}, t) = \frac{1}{2m}\left(-i\hbar\nabla - \frac{e}{c}\mathbf{A}_\lambda(\mathbf{x}, t)\right)^2 + V(\mathbf{x}). \tag{2.3}$$

We have not included the spin $\mathbf{S}$ of the electron, although it interacts with the magnetic field $\mathbf{B}$ and thus gives rise to the interaction term

$$H_S(\mathbf{x}, t) = -\frac{e}{m}\mathbf{S}\cdot\mathbf{B}(\mathbf{x}, t), \tag{2.4}$$

which has to be added to the Hamiltonian (2.3). We neglect this term because it is considerably smaller than the interaction term $H_I = \mathbf{A}_\lambda(\mathbf{x}, t)\cdot\mathbf{p}$. To see this, we consider a plane electromagnetic wave

$$\mathbf{A}_\lambda(\mathbf{x}, t) = A\left(e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)} + e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega t)}\right)\hat{\varepsilon}, \tag{2.5}$$

with amplitude A, frequency $\omega = \frac{2\pi c}{\lambda}$, wave vector $\mathbf{k}$ and polarization $\hat{\varepsilon}$, such that

$$|\mathbf{k}| = \frac{2\pi}{\lambda}, \quad \mathbf{k}\cdot\hat{\varepsilon} = 0.$$

The spin being of order $\hbar$ and the magnetic field $|\mathbf{B}| = |\nabla \times \mathbf{A}_\lambda| \sim |\mathbf{k}|A$, we conclude that (2.4) is of order $H_S \sim A\hbar|\mathbf{k}|$. Comparing this to H_I, we find

$$\frac{H_S}{H_I} \sim \frac{A\hbar|\mathbf{k}|}{A|\mathbf{p}|} \sim \frac{|\mathbf{x}|}{\lambda},$$

where we have used that $\frac{\hbar}{|\mathbf{p}|}$ is, due to the uncertainty relation, at most of order $|\mathbf{x}|$. For sufficiently large λ, this fraction becomes very small. We will see that it is of the same order of magnitude as the part of the interaction term which we neglect when performing the dipole approximation (2.6), hence we omit it from our description.

2.2 Hamiltonian in Dipole Approximation

In the usual experimental setup, the wavelength of the external field is much larger than the spatial extent of the region where the electron can move. We may therefore expand the vector potential $\mathbf{A}_\lambda(\mathbf{x}, t)$ in powers of $\mathbf{x}$, which yields a series of multipole moments of increasing order, and in good approximation keep only the lowest-order term $\mathbf{A}_\lambda(0, t)$. In the example of the plane wave (2.5), this is done by expanding the exponentials in a Taylor series in $\frac{|\mathbf{x}|}{\lambda}$,

$$\exp\left\{\pm i(\mathbf{k}\cdot\mathbf{x} - \omega t)\right\} = \exp\left\{\pm 2\pi i \frac{|\mathbf{x}|}{\lambda}\hat{k}\cdot\hat{x}\right\} e^{\mp i\omega t} \approx \left(1 + \mathcal{O}\left(\tfrac{|\mathbf{x}|}{\lambda}\right)\right) e^{\mp i\omega t}, \tag{2.6}$$

hence $\mathbf{A}_\lambda(\mathbf{x}, t) \approx \mathbf{A}_\lambda(0, t)$. Intuitively, this approximation is clear: as the Coulomb potential keeps the electron close, the external field can merely change insignificantly between electron and nucleus. Thus we can in good approximation discard the spatial change over the atom and assume instead that the electron interacts with a (spatially) constant electromagnetic field. The resulting semiclassical Hamiltonian in Coulomb gauge is

$$H_\infty(t) = \frac{1}{2m}\left(-i\hbar\nabla - \frac{e}{c}\mathbf{A}_\lambda(0, t)\right)^2 + V(\mathbf{x}). \tag{2.7}$$

If we had not truncated the multipole expansion of $\mathbf{A}_\lambda(\mathbf{x}, t)$ after the constant term, we would have obtained further terms such as the magnetic dipole moment, electric quadrupole moment etc. These are practically always negligible in comparison with the dipole term. They may however become important in the context of atomic transitions, when the dipole contribution to the transition probability vanishes in consequence of a selection rule[1].

The dipole approximation holds well for most experimental situations, but it is in the nature of an approximation to be of limited validity. First, its breakdown can clearly be expected when the wavelength becomes comparable to the target size. In practice there exists also a second limit towards long wavelengths. The external magnetic field in dipole approximation is zero because $\mathbf{B}(\mathbf{x}, t) = \nabla \times \mathbf{A}_\lambda(0, t) = 0$. This may however be an oversimplification if electrons of very high kinetic energy emerge from the interaction. They are strongly influenced by the magnetic field as the magnetic component of the Lorentz force depends on the electron's velocity. Sufficiently fast electrons are created in strong-field ionisation with very intense lasers and cause a breakdown of the dipole approximation in this regime [23]. In this

[1] For selection rules, see e.g. [2, Ch. 2.2]

thesis, we restrict ourselves to the description of non-relativistic electrons and therefore do not consider the second case. We will however rigorously confirm the first limit.

Although the Hamiltonian (2.7) is convenient for the mathematical analysis, the (physical) investigation of interaction processes is very often based on a different Hamiltonian,

$$\widetilde{H}(t) = \frac{\mathbf{p}^2}{2m} - e\mathbf{E}(0,t)\cdot\mathbf{x} + V(\mathbf{x}). \tag{2.8}$$

We will in the sequel show that $H_\infty(t)$ and $\widetilde{H}(t)$ are in fact related by a gauge transformation. To see this, we first consider the classical Hamiltonian (2.1) in dipole approximation. We use our freedom to choose a gauge for the vector and electrostatic potential by the simultaneous transform

$$\begin{cases} \mathbf{A}_\lambda(\mathbf{x},t) \to \widetilde{\mathbf{A}}_\lambda(\mathbf{x},t) = \mathbf{A}_\lambda(\mathbf{x},t) + \nabla\Lambda(\mathbf{x},t)\ , \\ \Phi(\mathbf{x},t) \to \widetilde{\Phi}(\mathbf{x},t) = \Phi(\mathbf{x},t) - \frac{1}{c}\frac{\partial}{\partial t}\Lambda(\mathbf{x},t)\ . \end{cases}$$

Our aim is to identify a transformation such that $\widetilde{\mathbf{A}}_\lambda(0,t) = 0$. This is achieved by the *Göppert-Mayer transformation*,

$$\Lambda(\mathbf{x},t) = -\mathbf{x}\cdot\mathbf{A}_\lambda(0,t),$$

which results in the transformed classical Hamiltonian

$$\widetilde{H}(\mathbf{x},\mathbf{p},t) = \frac{\mathbf{p}^2}{2m} - e\mathbf{E}(0,t)\cdot\mathbf{x} + V(\mathbf{x}).$$

Proceeding to the semiclassical Hamiltonian (2.7), we recall that, within the framework of quantum mechanics, a gauge transformation corresponds to a unitary transformation. Consequently, we seek a unitary operator $T(t)$ translating the operator $\mathbf{p}$ by $\frac{e}{c}\mathbf{A}_\lambda(0,t)$, i.e.

$$T(t)\mathbf{p}T(t)^\dagger = \mathbf{p} + \tfrac{e}{c}\mathbf{A}_\lambda(0,t).$$

This translation operator is naturally given by

$$T(t) = \exp\left\{-\tfrac{i}{\hbar}e\mathbf{A}_\lambda(0,t)\cdot\mathbf{x}\right\}. \tag{2.9}$$

Hence the wave function describing the electron transforms as

$$\widetilde{\psi}(t) = T(t)\psi(t),$$

which implies for the Schrödinger equation

$$i\hbar\partial_t\widetilde{\psi}(t) = \Big(T(t)H(t)T(t)^\dagger + i\hbar T(t)\left(\partial_t T(t)\right)T(t)^\dagger\Big)\,\widetilde{\psi}(t).$$

The operator $\widetilde{H}(t)$ generating the time evolution of $\widetilde{\psi}(t)$ is consequently given as

$$\widetilde{H}(t) = T(t)H(t)T(t)^\dagger + i\hbar T(t)\left(\partial_t T(t)\right)T(t)^\dagger.$$

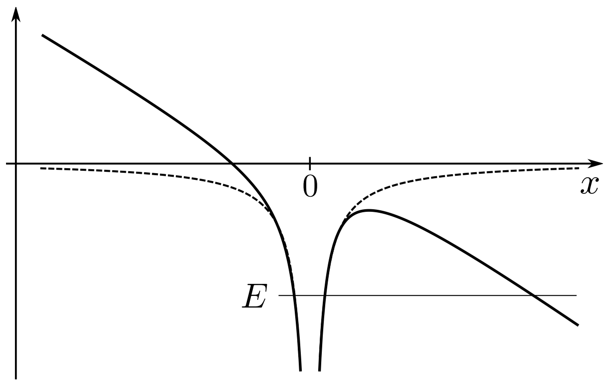

Figure 2.1: The effective potential $V_{\text{eff}}(\mathbf{x})$ in one dimension in comparison the undisturbed Coulomb potential (dashed line). The horizontal line indicates the energy E of an electron which may tunnel through the potential barrier (Figure taken from [13]).

With the explicit form (2.9) of $T(t)$, this yields precisely (2.8). The interaction $e\mathbf{E}(0,t)\cdot\mathbf{x}$ in (2.8) describes the coupling of the external field to the electric dipole moment $\mathbf{d} = e\mathbf{x}$ of the electron with respect to the origin – hence the term *dipole approximation*.

The Hamiltonian $\widetilde{H}(t)$ is particularly useful for descriptions of the ionisation of atoms as a consequence of interactions with light. Due to the incident radiation, the electron is no longer confined in the Coulomb potential $V(\mathbf{x}) = -e^2|\mathbf{x}|^{-1}$ but feels the effective potential

$$V_{\text{eff}}(\mathbf{x}) = -\frac{e^2}{|\mathbf{x}|} - e\mathbf{E}(0,t)\cdot\mathbf{x}.$$

Figure 2.1 shows $V_{\text{eff}}(\mathbf{x})$ for one dimension at a fixed instant of time. In comparison to the Coulomb potential it is deformed in such a way that the electron can tunnel through the potential barrier and escape the atom towards the impinging light.

Having motivated the dipole approximation heuristically, we proceed to the main part of the thesis: the proof in the semiclassical context. For this purpose, we continue with a chapter reviewing the concepts and theorems needed for a rigorous analysis.

3 Mathematical Preparations

In Chapter 4, we will consider the time evolution of wave functions under the exact Hamiltonian (2.3) as well as under the Hamiltonian in dipole approximation (2.7). Both being unbounded, we need to agree upon some definitions and introduce several concepts related to unbounded operators, including questions of domain and self-adjointness. In so doing, we will follow [24, 25, 26, 14, 27, 28, 29, 30].
In order to prove the self-adjointness of the free Schrödinger operator, we define the Fourier transform on $L^2(\mathbb{R}^d)$ and introduce the notion of Sobolev spaces. This part of the chapter refers to [27, 30, 31].
Subsequently, we introduce $\mathcal{C}_0$-semigroups and examine their generators. The most important results in this section are the theorems by Hille and Yosida and by Stone. Our presentation is based on [15, 16, 32, 33, 34].
We then establish existence and uniqueness of the time evolution for explicitly time-dependent unbounded Hamiltonians. The main references for this are [24, 25, 15, 16, 35, 36].
In the last section, we introduce the Gronwall inequality, following [37, 38].
All theorems, lemmas, proofs and definitions in this chapter are copied from said references. The only exceptions are the proofs of Lemmas 3.4, 3.7, 3.22 and 3.37. In Section 3.4, we present the proofs of the respective theorems as they are given in the quoted literature, although in considerably greater detail. The proofs of Theorem 3.42, Lemma 3.43 and Theorem 3.45 are marginally altered to include the case $T \neq 1$.

3.1 Unbounded Operators

A **(linear) operator** A is a linear map

$$A : X \supseteq \mathcal{D}(A) \to Y$$

from a normed vector space X into a normed vector space Y, whose domain $\mathcal{D}(A)$ is a subspace of X. If $\mathcal{D}(A)$ is dense with respect to the norm of X, A is called **densely defined**. If $X = Y$, we call A an **operator on X**. Quantum mechanics deals with operators on a Hilbert space $\mathcal{H}$.
If Y is a subspace of X, an operator A on X induces a linear operator A' on Y such that

$$\mathcal{D}(A') = \{x \in \mathcal{D}(A) \cap Y : Ax \in Y\},$$

$$A'x = Ax \quad \forall\, x \in \mathcal{D}(A').$$

This operator A' is called the **part of A on Y**.

Later in this thesis we will be concerned with a family of bonded operators (Lemma 3.40). A useful characteristic of such families is their total variation.

Definition 3.1. *A family* $\{A(t)\}_{t\in[a,b]}$ *of operators on a Banach space* X *is called* ***of bounded variation*** *in* t *if there is some* $N \geq 0$ *such that*

$$\sum_{j=1}^{n} \|A(t_j) - A(t_{j-1})\|_X \leq N$$

for every partition $a = t_0 < t_1 < \cdots < t_n = b$ *of the interval* $[a, b]$. *The smallest such* N *is called the* ***total variation*** *of* A *in* t.

In quantum mechanics, the statistics of measurements are described by means of self-adjoint operators. A brief justification of this particular choice will be given in Section 3.4; for now, we merely define self-adjointness.

Definition 3.2. *For a densely defined operator* A *on* $\mathcal{H}$, *its* ***adjoint*** A^* *is defined by*

$$\mathcal{D}(A^*) := \big\{\psi \in \mathcal{H} : \exists\, \eta_\psi \in \mathcal{H} \text{ s.t. } \langle\psi, A\varphi\rangle = \langle\eta_\psi, \varphi\rangle \;\forall \varphi \in \mathcal{D}(A)\big\},$$

$$A^*\psi := \eta_\psi.$$

(a) *A is called* ***symmetric*** *if* $\langle\psi, A\varphi\rangle = \langle A\psi, \varphi\rangle \;\forall\, \psi, \varphi \in \mathcal{D}(A)$, *and* ***skew symmetric*** *if* $\langle\psi, A\varphi\rangle = -\langle A\psi, \varphi\rangle \;\forall\, \psi, \varphi \in \mathcal{D}(A)$.

(b) *A is called* ***self-adjoint*** *if* $A = A^*$, *which in particular requires* $\mathcal{D}(A) = \mathcal{D}(A^*)$, *and* ***skew self-ajoint*** *if* $A = -A^*$.

Whereas for bounded operators the notions *symmetric* and *self-adjoint* are equivalent, this is not true for unbounded operators. A symmetric operator is not automatically self-adjoint, it is merely extended by its adjoint.
The requirement that $\mathcal{D}(A)$ be dense ensures the well-definedness of A^*. $\mathcal{D}(A^*)$ need not be dense in general, it might even contain no element besides 0. Finding the domain of self-adjointness of an operator is therefore a balancing procedure: increasing the domain of A implies decreasing the domain of A^*. It is in general not trivial to determine whether an operator is self-adjoint. In preparation for a very useful criterion of self-adjointness (Theorem 3.5), we introduce the concept of closed operators.

Definition 3.3. *The* ***graph*** *of an operator* $A : X \supseteq \mathcal{D}(A) \to Y$, X *and* Y *being two normed spaces, is defined as the set*

$$\Gamma(A) := \big\{(\varphi, A\varphi) : \varphi \in \mathcal{D}(A)\big\} \subseteq X \times Y.$$

The ***graph norm*** *of* A *is defined as*

$$\|\cdot\|_A := \|\cdot\|_X + \|A\,\cdot\|_Y\,.$$

A is called ***closed*** *if* $\Gamma(A)$ *is closed in* $(X \times Y, \|\cdot\|_{X\times Y})$, *where* $\|(x, y)\|_{X\times Y} = \|x\|_X + \|y\|_Y$. *This is equivalent to the following condition:*

$$\Big\{\{\varphi_n\}_{n\in\mathbb{N}} \subset \mathcal{D}(A),\, \lim_{n\to\infty} \varphi_n = \varphi \text{ and } \lim_{n\to\infty} A\varphi_n = \psi\Big\} \implies \Big\{\varphi \in \mathcal{D}(A) \text{ and } A\varphi = \psi\Big\}.$$

Closed operators display a useful property: their domain endowed with their graph norm forms a Banach space.

Lemma 3.4. *Let $A : X \supseteq \mathcal{D}(A) \to Y$ be a linear map between two Banach spaces X and Y. Then*

$$A \text{ is closed } \iff (\mathcal{D}(A), \|\cdot\|_A) \text{ is a Banach space.}$$

Proof. Let $\varphi \in \mathcal{D}(A)$ and $\{\varphi_n\}_{n\in\mathbb{N}}$ a sequence in $\mathcal{D}(A)$. As

$$\|(\varphi, A\varphi)\|_{X\times Y} = \|\varphi\|_X + \|A\varphi\|_Y = \|\varphi\|_A \,,$$

$\{(\varphi_n, A\varphi_n)\}_{n\in\mathbb{N}}$ is a Cauchy sequence in $(\Gamma(A), \|\cdot\|_{X\times Y})$ precisely if $\{\varphi_n\}_{n\in\mathbb{N}}$ is a Cauchy sequence in $(\mathcal{D}(A), \|\cdot\|_A)$. Hence $(\mathcal{D}(A), \|\cdot\|_A)$ is complete if and only if $\Gamma(A)$ is complete with respect to $\|\cdot\|_{X\times Y}$. The claim follows because completeness is equivalent to closedness for subspaces of Banach spaces. □

Now we can state said criterion of self-adjointness.

Theorem 3.5. *For a symmetric operator A on $\mathcal{H}$, the following are equivalent:*

(a) *A is self-adjoint,*

(b) *A is closed and* $\operatorname{Ker}(A^* \pm i\mathbb{1}) = \{0\}$,

(c) $\operatorname{Ran}(A \pm i\mathbb{1}) = \mathcal{H}$.

Proof. [26], Theorem VIII.3. □

How much may one perturb a self-adjoint operator without losing its self-adjointness on the original domain? In Section 3.2, we will see that the Laplace operator $-\Delta$, describing the free evolution of a particle, is self-adjoint. As the Hamiltonians (2.3) and (2.7) are of the form $-\Delta + V$, we introduce a criterion on V ensuring the self-adjointness of the sum (Theorem 3.8). Therefore we need the notion of relative boundedness.

Definition 3.6. *Let A and B be two densely defined operators on a Hilbert space $\mathcal{H}$. Suppose that*

(i) $\mathcal{D}(B) \supseteq \mathcal{D}(A)$,

(ii) *there exist $a, b \in \mathbb{R}$ such that for all $\varphi \in \mathcal{D}(A)$,*

$$\|B\varphi\| \le a\,\|A\varphi\| + b\,\|\varphi\| \,. \tag{3.1}$$

*Then B is called **(relatively) A-bounded**. The infimum of such a is called the **relative bound** of B with respect to A, or simply the **A-bound** of B. If the relative bound is zero, B is called **infinitesimally A-bounded**, and we denote this by $B << A$.*

Sometimes it may be more convenient to cope with a slightly different condition than (3.1):

Lemma 3.7. *Condition (ii) can be replaced by the equivalent condition*

(ii') *there exist $\tilde{a}, \tilde{b} \in \mathbb{R}$ such that for all $\varphi \in \mathcal{D}(A)$,*

$$\|B\varphi\|^2 \le \tilde{a}^2\,\|A\varphi\|^2 + \tilde{b}^2\,\|\varphi\|^2 \,. \tag{3.2}$$

The infimum over all a in (ii) equals the infimum over all $\tilde{a}$ in (ii').

Proof. Suppose (ii') holds. Then

$$\|B\varphi\|^2 \le \tilde{a}^2 \|A\varphi\|^2 + \tilde{b}^2 \|\varphi\|^2 \le \left(\tilde{a}\,\|A\varphi\| + \tilde{b}\,\|\varphi\|\right)^2,$$

hence

$$\|B\varphi\| \le \tilde{a}\,\|A\varphi\| + \tilde{b}\,\|\varphi\|,$$

and we choose $a = \tilde{a}$, $b = \tilde{b}$. The respective infima are trivially equal.
Conversely, suppose (ii) holds. Then

$$\|B\varphi\|^2 \le a^2 \|A\varphi\|^2 + b^2 \|\varphi\|^2 + 2a\sqrt{\varepsilon}\,\|A\varphi\| \cdot b\tfrac{1}{\sqrt{\varepsilon}}\,\|\varphi\|$$

for all $\varepsilon > 0$. Using the identity $2cd \le c^2 + d^2$ for $c, d \in \mathbb{R}$, we conclude

$$\|B\varphi\|^2 \le a^2(1+\varepsilon)\,\|A\varphi\|^2 + b^2(1+\tfrac{1}{\varepsilon})\,\|\varphi\|^2$$

and choose $\tilde{a}^2 = (1+\varepsilon)a^2$, $\tilde{b}^2 = (1+\frac{1}{\varepsilon})b^2$. As this can be done for arbitrary $\varepsilon > 0$, the infimum over all possible a equals the infimum over all possible $\tilde{a}$. □

After this preparatory work we present a quite renowned theorem providing us with a useful tool for the construction of self-adjoint operators.

Theorem 3.8. (Kato, Rellich) *Let A, B be operators on a Hilbert space $\mathcal{H}$. Suppose that A is self-adjoint and B is symmetric with A-bound $a < 1$. Then $A + B$ is self-adjoint on $\mathcal{D}(A+B) = \mathcal{D}(A)$.*

Proof. [27], Theorem 6.4. □

This theorem has an extension concerning the lower bound of $A + B$.

Definition 3.9. *A self-adjoint operator A on a Hilbert space $\mathcal{H}$ is called **semibounded** if there exists $\gamma_A \in \mathbb{R}$ such that $\langle \varphi, A\varphi \rangle \ge \gamma_A \|\varphi\|^2$ for each $\varphi \in \mathcal{D}(A)$. Each such γ_A is called a **lower bound** for A.*

We may choose for φ elements from the spectral basis of A. As A has in this basis diagonal form, the spectrum must be lower bounded by γ_A, which explains the term *lower bound*. Making use of Theorem 3.8 it is also possible to find a lower bound γ on the sum $A + B$, which is however in general not the ideal choice.

Theorem 3.10. *Let A, B be operators on a Hilbert space $\mathcal{H}$. Let A be self-adjoint and semibounded with lower bound γ_A, and let B be symmetric and relatively A-bounded with A-bound $a < 1$. Then $A + B$ is semibounded with lower bound*

$$\gamma = \gamma_A - \max\left\{\frac{b}{1-a},\, b + a|\gamma_A|\right\},$$

with a and b as in Definition 3.6.

Proof. [28], Satz 9.7. □

To conclude the paragraph on perturbations of self-adjoint operators, we introduce the HEINZ inequality.

Lemma 3.11. (HEINZ) *Let A be a positive self-adjoint operator on a Hilbert space $\mathcal{H}$ and let B be symmetric with $\mathcal{D}(A) \subseteq \mathcal{D}(B)$. If*

$$\|B\varphi\| \leq \|A\varphi\| \qquad \forall \varphi \in \mathcal{D}(A)$$

then

$$|\langle \varphi, B\varphi \rangle| \leq \langle \varphi, A\varphi \rangle \qquad \forall\, \varphi \in \mathcal{D}(A).$$

Proof. [28], Satz 9.9. □

An important characteristic of an unbounded operator is its resolvent set: the subset of $\mathbb{C}$ on which the operator is invertible. Its complement, the spectrum, is a generalisation of the set of eigenvectors of a matrix.

Definition 3.12. *Let A be a closed operator on a Banach space X. A complex number λ is contained in the* ***resolvent set*** *$\rho(A)$ if $\lambda\mathbb{1} - A : X \supseteq \mathcal{D}(A) \to X$ is a bijection with bounded inverse.*
If $\lambda \in \rho(A)$,

$$R_\lambda(A) := (\lambda\mathbb{1} - A)^{-1} \in \mathcal{L}(X)$$

is called the ***resolvent*** *of A at λ.*

Especially in Chapter 4 we will extensively work with resolvents, hence we introduce now two identities which will simplify our arguments.

Theorem 3.13. *Let A be a closed densely defined operator. Then $\{R_\lambda(A) : \lambda \in \rho(A)\}$ is a commuting family of bounded operators satisfying the* ***first resolvent identity****,*

$$R_\lambda(A) - R_\mu(A) = (\mu - \lambda)R_\mu(A)R_\lambda(A). \tag{3.3}$$

If additionally $\mathcal{D}(A) = \mathcal{D}(B)$, the ***second resolvent identity****,*

$$R_\lambda(A) - R_\lambda(B) = R_\lambda(A)(A - B)R_\lambda(B) = R_\lambda(B)(A - B)R_\lambda(A), \tag{3.4}$$

holds for $\lambda \in \rho(A) \cap \rho(B)$.

Proof. [28], Satz 5.4. □

Let us finally generalise the concept of commutativity to unbounded operators.

Definition 3.14. *Let A, B be two self-adjoint operators on a Hilbert space $\mathcal{H}$. Then A and B are said to* ***commute*** *if all projections in their associated projection-valued measures commute.*

It is necessary to make this detour via the projection-valued measures because the expression $AB - BA$ might not be sensible for any vector in $\mathcal{H}$: it may very well happen that

$$\mathrm{Ran}(A) \cap \mathcal{D}(B) = \{0\},$$

in which case BA has no meaning.

3.2 Free Schrödinger Operator

In this section, we define the free Schrödinger operator $H_0 = -\Delta$ and establish its self-adjointness. To this end, we introduce the Fourier transform on $L^2(\mathbb{R}^d)$, which is a useful tool as it permits the reduction of differential operators to simple multiplication operators. We cannot define it directly on $L^2(\mathbb{R}^d)$ because $f(\mathbf{x})e^{-i\mathbf{k}\cdot\mathbf{x}}$ is in general not integrable for $f \in L^2(\mathbb{R}^d)$. Therefore we take a detour over $\mathcal{S}(\mathbb{R}^d)$ and extend in a second step to $L^2(\mathbb{R}^d)$.

Definition 3.15. *The **Fourier transform** on Schwartz space is defined as*

$$\begin{aligned} \mathcal{F} : \mathcal{S}(\mathbb{R}^d) &\longrightarrow \mathcal{S}(\mathbb{R}^d) \\ f &\longmapsto \mathcal{F}(f) \equiv \widehat{f}, \end{aligned}$$

where

$$\widehat{f}(\mathbf{p}) := (2\pi)^{-\frac{d}{2}} \int\limits_{\mathbb{R}^d} f(\mathbf{x}) e^{-i\mathbf{p}\cdot\mathbf{x}} d\mathbf{x}. \tag{3.5}$$

Theorem 3.16. *The Fourier transform has the following properties:*

(a) $\mathcal{F} : \mathcal{S}(\mathbb{R}^d) \longrightarrow \mathcal{S}(\mathbb{R}^d)$ is a bijection, and its inverse is given by

$$\mathcal{F}^{-1}(g)(\mathbf{x}) \equiv \breve{g}(\mathbf{x}) = (2\pi)^{-\frac{d}{2}} \int\limits_{\mathbb{R}^d} g(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} d\mathbf{p},$$

(b) $\mathcal{F}$ extends to a unitary operator $\mathcal{F} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$,

(c) in particular, for all $f, g \in L^2(\mathbb{R}^d)$,

$$\|f\|_2 = ||\hat{f}||_2,$$

$$\langle f, g \rangle_{L^2(\mathbb{R}^d)} = \langle \hat{f}, \hat{g} \rangle_{L^2(\mathbb{R}^d)}.$$

Proof. [27], Chapter 7.1, Theorems 7.4 and 7.5. □

Part (c) is also known as as PLANCHEREL's identity. As mentioned above, one major benefit of the Fourier transform is that it provides us with the possibility to treat differential operators as multiplication operators. This feature is caught by the subsequent lemma.

Lemma 3.17. *For $f \in \mathcal{S}(\mathbb{R}^d)$ and a multi-index $\alpha \in \mathbb{N}_0^n$, we have*

$$\partial_\alpha f(\mathbf{x}) = [(i\mathbf{p})^\alpha \widehat{f}]^\vee(\mathbf{x})$$

for all partial derivatives ∂_α with $|\alpha| \leq k$.

Proof. [27], Chapter 7.1, Lemma 7.1. □

Hence the free Schrödinger operator $-\Delta$ acts in Fourier space as multiplication operator $|\cdot|^2$. Its domain is consequently constituted of all those $f \in L^2(\mathbb{R}^d)$ for which $\| |\cdot|^2 \widehat{f}||$ exists. This leads us to the notion of Sobolev spaces.

Definition 3.18. *Consider an open set $\Omega \subseteq \mathbb{R}^d$, $k \geq 0$. The* ***(Hilbert-)Sobolev space*** *$H^k(\Omega)$ is defined as*

$$H^k(\Omega) := \{f \in L^2(\Omega) : (1 + |\cdot|^2)^{\frac{k}{2}} \widehat{f} \in L^2(\Omega)\}. \tag{3.6}$$

By Theorem 3.16, Lemma 3.17 can thus be extended to $f \in H^k(\mathbb{R}^d)$, where $\partial_\alpha f$ is the derivative of f in the sense of distributions.

Theorem 3.19. *$H^k(\Omega)$ with the scalar product*

$$\langle f, g \rangle_{H^k(\Omega)} := \int\limits_{\Omega} \overline{\widehat{f}(\mathbf{p})} \widehat{g}(\mathbf{p})(1 + |\mathbf{p}|^2)^k d\mathbf{p} \tag{3.7}$$

is a Hilbert space.

Proof. [31], Theorem 3.5. □

The scalar product (3.7) induces the **Sobolev norm**

$$\|f\|^2_{H^k(\Omega)} = \int\limits_{\Omega} (1 + |\mathbf{p}|^2)^k |\widehat{f}(\mathbf{p})|^2 d\mathbf{p}. \tag{3.8}$$

In particular, the norm on $H^2(\mathbb{R}^d)$ is given by

$$\begin{aligned} \|f\|^2_{H^2(\mathbb{R}^d)} &= \int\limits_{\mathbb{R}^d} |\widehat{f}(\mathbf{p})|^2 d\mathbf{p} + 2 \int\limits_{\mathbb{R}^d} |\mathbf{p}\widehat{f}(\mathbf{p})|^2 d\mathbf{p} + \int\limits_{\mathbb{R}^d} |\mathbf{p}^2 \widehat{f}(\mathbf{p})|^2 d\mathbf{p} \\ &= \|f\|_2^2 + 2 \left\| |\cdot| \widehat{f} \right\|_2^2 + \left\| |\cdot|^2 \widehat{f} \right\|_2^2. \end{aligned} \tag{3.9}$$

As the norms of $|\cdot|\widehat{f}$ and $|\cdot|^2\widehat{f}$ will appear quite frequently, we introduce the more compact notation

$$\begin{aligned} \|\nabla f\|_2^2 &:= \left\| |\cdot| \widehat{f} \right\|_2^2 = \sum_{i=1}^{d} \int\limits_{\mathbb{R}^d} |\partial_i f(\mathbf{x})|^2 d\mathbf{x}, \\ \|\Delta f\|_2^2 &:= \left\| |\cdot|^2 \widehat{f} \right\|_2^2 = \int\limits_{\mathbb{R}^d} |\Delta f(\mathbf{x})|^2 d\mathbf{x}. \end{aligned}$$

In this notation, (3.9) leads immediately to the following corollary.

Corollary 3.20. *Let $f \in H^2(\mathbb{R}^d)$. Then*

$$\|f\| \leq \|f\|_{H^2(\mathbb{R}^d)}, \tag{3.10}$$

$$\|\nabla f\| \leq \tfrac{1}{2} \|f\|_{H^2(\mathbb{R}^d)}, \tag{3.11}$$

$$\|-\Delta f\| \leq \|f\|_{H^2(\mathbb{R}^d)}. \tag{3.12}$$

We enclose two lemmas concerning dense embeddings.

Lemma 3.21. *$\mathcal{C}_c^\infty(\mathbb{R}^d)$ is dense in $H^k(\mathbb{R}^d)$.*

Proof. [31], Theorem 7.38. □

Lemma 3.22. *$H^k(\Omega)$ is dense in $L^2(\Omega)$.*

Proof. It is well known from functional analysis that $\mathcal{C}_c^\infty(\Omega)$ is dense in $L^p(\Omega)$ for $1 \leq p < \infty$ (e.g. [27], Theorem 0.33). Further, $\mathcal{C}_c^\infty(\mathbb{R}^d)$ is dense in $H^k(\Omega)$ by Lemma 3.21. Thus $H^k(\Omega)$ is a subset and contains a dense subset of $L^2(\Omega)$, which makes it a dense subset itself. □

Finally, the following theorem proves the self-adjointness of the free Schrödinger operator on the Sobolev space $H^2(\mathbb{R}^d)$, and thus concludes the current section.

Theorem 3.23. *The free Schrödinger Operator $H_0 = -\Delta$ is positive and self-adjoint on $\mathcal{D}(H_0) = H^2(\mathbb{R}^d)$.*

Proof. [27], Theorem 7.7. □

3.3 Semigroups and their Generators

This section is meant to provide the basis for Section 3.4, which is concerned with the time evolution generated by an unbounded, time-dependent Hamiltonian. Especially Theorem 3.38 makes ample use of notions from the theory of semigroups, hence we will give a short overview over the concepts involved.
One may think of semigroups as the generalisation of exponential functions to Banach spaces: semigroups arise as the solutions of ordinary differential equations with constant coefficients in Banach spaces, in the same way as exponential functions do in $\mathbb{C}$.

Definition 3.24. *Let X be a Banach space. A one-parameter family $\{T(t)\}_{0\leq t<\infty} \subseteq \mathcal{L}(X)$ is called a **semigroup of class** $\mathcal{C}_0$, or simply a $\mathcal{C}_0$**-semigroup** (or a **strongly continuous semigroup**), on X, if*

(i) $T(0) = \mathbb{1}$,

(ii) $T(t+s) = T(t)T(s) \;\; \forall\, t, s \geq 0$ *(semigroup property),*

(iii) $\operatorname*{s-lim}_{t\to t_0} T_t = T_{t_0}$.

A $\mathcal{C}_0$-semigroup is thus a strongly continuous one-parameter group where the parameter attains only non-negative values. The norm of the elements of a $\mathcal{C}_0$-semigroup grows at most exponentially in the parameter.

Theorem 3.25. *Let $\{T(t)\}$ be a $\mathcal{C}_0$-semigroup on X. Then there exist constants $\beta \geq 0$ and $M \geq 1$ such that*

$$\|T(t)\|_X \leq M e^{\beta t} \;\; \forall\, 0 \leq t < \infty.$$

Proof. [32], Chapter I, Theorem 2.2. □

If $\beta = 0$, $\{T(t)\}$ is uniformly bounded. A special case of uniformly bounded semigroups are the contraction semigroups.

Definition 3.26. *Let $\{T(t)\}$ be a $\mathcal{C}_0$-semigroup . If $\beta = 0$ and $M = 1$ (with β and M as in Theorem 3.25), it is called a* ***contraction semigroup****.*

Keeping in mind the parallel to exponential functions, we now examine the generators of $\mathcal{C}_0$-semigroups.

Definition 3.27. *The* ***(infinitesimal) generator*** *A of a $\mathcal{C}_0$-semigroup $\{T(t)\}$ on X is defined as*

$$\begin{aligned} A &= \operatorname*{s-lim}_{t \downarrow 0} \frac{T(t) - \mathbb{1}}{t}, \\ \mathcal{D}(A) &= \left\{ \psi \in X : \lim_{t \downarrow 0} \frac{T(t) - \mathbb{1}}{t} \psi \text{ exists in } X \right\}. \end{aligned}$$

We denote by $\mathcal{G}(X, M, \beta)$ the set of all A such that $-A$ generates a $\mathcal{C}_0$-semigroup on X with constants M and β[1]. Further,

$$\mathcal{G}(X) := \bigcup_{\beta \in \mathbb{R}} \bigcup_{M > 0} \mathcal{G}(X, M, \beta).$$

Theorem 3.28. *The generator of a $\mathcal{C}_0$-semigroup is closed and densely defined and determines the semigroup uniquely.*

Proof. [33], Chapter II, Theorem 1.4. □

Naturally the generator commutes with every element of the $\mathcal{C}_0$-semigroup it generates.

Theorem 3.29. *Let X be a Banach space and A the generator of a $\mathcal{C}_0$-semigroup $\{T(t)\}$. Then*

$$AT(t)\psi = T(t)A\psi = \lim_{h \to 0} \tfrac{1}{h}(T(t+h) - T(t))\psi.$$

Proof. [16], Chapter IX.3, Theorem 2. □

We state now two theorems characterising generators of $\mathcal{C}_0$-semigroups. The first theorem is concerned with the generator of generic $\mathcal{C}_0$-semigroups, the second specialises to contraction semigroups.

Theorem 3.30. *Let X be a Banach space. Then the operator A generates a $\mathcal{C}_0$-semigroup with constants M and β as defined in Theorem 3.25 if and only if*

(i) A is closed and densely defined,

(ii) $\|R_\lambda(A)^n\|_X \le M(\lambda - \beta)^{-n}$ for $\lambda > \beta$, $n = 1, 2, \dots$.

Proof. [32], Chapter I, Theorem 5.3. □

Theorem 3.31. (Hille, Yosida) *For an operator A on a Banach space X, the following are equivalent:*

[1] The definition with minus sign might at first glance appear awkward. The reason for this seemingly complicated convention is that we will make use of $\mathcal{G}(X, M, \beta)$ to solve the evolution equation in the form (3.20). Had we chosen to write it in the form (3.40), we would have defined $\mathcal{G}(X, M, \beta)$ with a plus sign.

(a) A generates a contraction semigroup,

(b) A is densely defined and closed. Moreover, $(0,\infty) \subseteq \rho(A)$ *and*

$$\|R_\lambda(A)\|_X \leq \frac{1}{\lambda}\ , \ \ \lambda > 0,$$

(c) A is densely defined and closed. Moreover, $\{\lambda \in \mathbb{C} : \Re(\lambda) > 0\} \subseteq \rho(A)$ *and*

$$\|R_\lambda(A)\|_X \leq \frac{1}{\Re(\lambda)}\ , \ \ \Re(\lambda) > 0.$$

Proof. [33], Chapter II, Theorem 3.5. □

The next theorem we present is presumably one of the most renowned theorems in quantum mechanics. It provides the connection between self-adjoint operators and unitary groups.

Theorem 3.32. (Stone) *Let* $\{U(t)\}_{t\in\mathbb{R}}$ *be a strongly continuous one-parameter group of unitary operators on* $\mathcal{H}$*. Then the infinitesimal generator of* $\{U(t)\}_{t\in\mathbb{R}}$ *is* $A = iH$*, with* H *a self-adjoint operator on* $\mathcal{H}$*.*
Conversely, if H *is a self-adjoint operator on* $\mathcal{H}$*, then* iH *generates a unique strongly continuous unitary one-parameter group* $\{e^{itH}\}_{t\in\mathbb{R}}$*.*

Proof. [33], Theorem 3.24. □

We come now to a number of definitions due to Kato [15], which we will need in the theorems of the ensuing section. The first is the notion of a subspace being admissible with respect to the generator of a $\mathcal{C}_0$-semigroup.

Definition 3.33. *Let* Y *be a Banach space which is densely and continuously embedded in a Banach space* X*, and let* $A \in \mathcal{G}(X, M, \beta)$*.* Y *is called **admissible with respect to** A, or simply A-**admissible**, if* $\{e^{-tA}\}_{0\leq t<\infty}$ *leaves* Y *invariant and forms a* $\mathcal{C}_0$*-semigroup on* Y*.*

Lemma 3.34. *Let* S *be an isomorphism of* Y *onto* X*. Then* Y *is* A*-admissible if and only if* $A_1 = SAS^{-1}$ *belongs to* $\mathcal{G}(X)$*. In this case,* $Se^{-tA}S^{-1} = e^{-tA_1}$ *for* $t \geq 0$*.*

Proof. [15], Proposition 2.4. □

Now we consider a whole family of generators of $\mathcal{C}_0$-semigroups. In this context, we define the notion of stability:

Definition 3.35. *Let* X *be a Banach space and consider the family* $\{A(t)\}_{0\leq t\leq T} \in \mathcal{G}(X)$*.* $\{A(t)\}$ *is called **stable** if there are constants* $M \geq 0$ *and* $\beta \in \mathbb{R}$ *such that*

$$\left\| \prod_{j=1}^{k} R_\lambda(-A(t_j)) \right\|_X \leq M(\lambda - \beta)^{-k}\ , \ \ \lambda > \beta, \tag{3.13}$$

for any finite family $\{t_j\}_{1\leq j\leq k}$ *with* $0 \leq t_1 \leq \cdots \leq t_k \leq T$*,* $k = 1, 2, \ldots$ *. The product* $\prod$ *is time-ordered, i.e. factors with larger* t_j *stand left of the factors with smaller* t_j*.* M *and* β *are called the **constants of stability**.*

Note that the constants M and β need not coincide with the constants of Theorem 3.25.

Lemma 3.36. *Condition (3.13) is equivalent to the condition*

$$\left\| \prod_{j=1}^{k} e^{-s_j A(t_j)} \right\|_X \leq M e^{\beta(s_1+\cdots+s_k)} , \quad s_j \geq 0, \tag{3.14}$$

for $\{t_j\}_{1\leq j\leq k}$ *and* $\prod$ *as above.*

Proof. [15], Proposition 3.3. □

It can easily be seen that the generators of contraction semigroups are inherently stable.

Lemma 3.37. *Let* $-A(t)$ *be a generator of a contraction semigroup for* $t \in [0,T]$*. Then the family* $\{A(t)\}$ *is stable with constants of stability* $M = 1$ *and* $\beta = 0$*.*

Proof. From the Hille-Yosida theorem (Theorem 3.31) we know that $(0,\infty) \subseteq \rho(A(t_j))$, and consequently $\|R_\lambda(-A(t_j))\| \leq \frac{1}{\lambda}$ for $\lambda > 0$, $t_j \in [0,T]$. The resolvents are bounded operators, hence their operator norms are submultiplicative. Therefore

$$\left\| \prod_{j=1}^{k} R_\lambda(-A(t_j)) \right\|_X \leq \prod_{j=1}^{k} \|R_\lambda(-A(t_j))\|_X \leq \lambda^{-k} \quad \forall \lambda > 0$$

for all finite families $\{t_j\}$ as specified in Definition 3.35. □

3.4 Time Evolution

Starting from an initial wave function $\psi(t_0)$, the solutions of the Schrödinger equation

$$i\partial_t \psi(t) = H(t)\psi(t) \tag{3.15}$$

should be uniquely determined and exist for all times. Further, we demand that the total probability $\|\psi(t)\|^2$ be conserved. These three requirements are met if the Schrödinger flow on the space of wave functions is described by a unitary strongly continuous one-parameter group $\{U(t,t_0)\}_{t\in\mathbb{R}}$ satisfying

$$i\partial_t U(t,t_0) = H(t)U(t,t_0). \tag{3.16}$$

We call this family of operators the **time evolution**.

But does H always generate a flow of this kind? In other words, is H necessarily the generator of a unitary group? The functional form of H is dictated by physics, but we are free to choose suitable boundary conditions – equivalently, to specify an appropriate domain for H. We note first that, in order to conserve probability, H must be symmetric as a consequence of the continuity equation[2]. Hence we must not choose the domain too small in order to preserve symmetry. If we choose it however too big, we might lose the uniqueness of the

[2] The continuity equation, also known as the quantum flux equation, is defined and motivated in [24], Chapter 7.

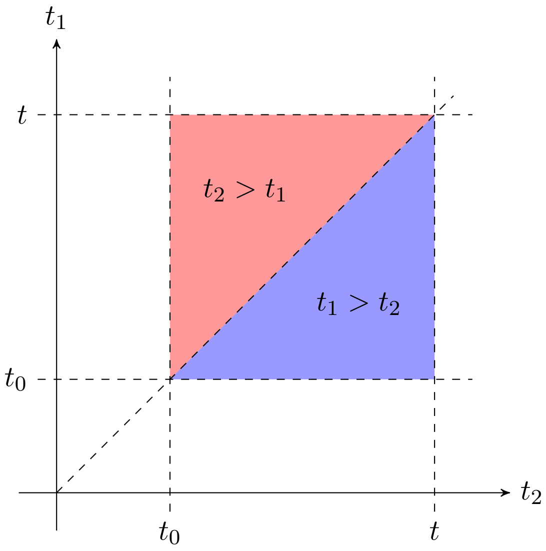

Figure 3.1: Regions of integration for $n = 2$. In the first two lines of (3.19), we integrate over the blue triangle whereas in the following lines the integration is performed over both the red and the blue segment. The segments have identical size.

solution. It turns out that the only possible choice is the domain on which H is self-adjoint[3].

The precise form of the time evolution operator depends on H. Let us first consider the simplest case where H is not (explicitly) time-dependent, for instance $H = -\Delta + V$. The time evolution is then determined by STONE's theorem (Theorem 3.32), and the unique solution of (3.16) is

$$U(t, t_0) = e^{-iH(t-t_0)}.$$

The situation becomes more involved if the Hamiltonian is explicitly time-dependent. One distinguishes three cases:
If $H(t)$ is bounded for any t and the $H(t)$ commute pairwise, i.e. $[H(t_1), H(t_2)] = 0$ for all t_1, t_2, the time evolution is given as

$$U(t, t_0) = e^{-i\int_{t_0}^{t} H(\tau)d\tau}. \tag{3.17}$$

More generally, if we impose on $H(t)$ to be still bounded but renounce the demand for pairwise commutativity, $U(t, t_0)$ is determined by the Dyson expansion,

$$\begin{aligned} U(t, t_0)\psi = \psi - i\int_{t_0}^{t} H(t_1)\psi \, dt_1 + (-i)^2 \int_{t_0}^{t}\int_{t_0}^{t_1} H(t_1)H(t_2)\psi \, dt_2 \, dt_1 \\ +(-i)^3 \int_{t_0}^{t}\int_{t_0}^{t_1}\int_{t_0}^{t_2} H(t_1)H(t_2)H(t_3)\psi \, dt_3 \, dt_2 \, dt_1 + \dots \; . \end{aligned} \tag{3.18}$$

[3]The full argument can be found in [24], Chapter 14.

(3.17) arises from (3.18) if the Hamiltonians commute. To see this, let S_n denote the set of permutations σ of $\{1, \ldots n\}$ and define

$$E_\sigma := \big\{(t_1, t_2, \ldots, t_n) : t \geq t_{\sigma(1)} \geq t_{\sigma(2)} \geq \cdots \geq t_{\sigma(n)} \geq t_0\big\}.$$

Due to the pairwise commutativity of $H(t)$ we obtain

$$\begin{aligned}
\int_{t_0}^{t}\int_{t_0}^{t_1} \cdots \int_{t_0}^{t_{n-1}} & H(t_1)H(t_2)\cdots H(t_n)\psi \, dt_n \cdots dt_2 \, dt_1 \\
&= \int_{E_{\mathrm{id}}} H(t_1)H(t_2)\cdots H(t_n)\psi \, dt_n \cdots dt_2 \, dt_1 \\
&= \frac{1}{n!} \sum_{\sigma \in S_n} \int_{E_\sigma} H(t_1)H(t_2)\cdots H(t_n)\psi \, dt_n \cdots dt_2 \, dt_1 \qquad (3.19)\\
&= \frac{1}{n!} \int_{t_0}^{t}\int_{t_0}^{t} \cdots \int_{t_0}^{t} H(t_1)H(t_2)\cdots H(t_n)\psi \, dt_n \cdots dt_2 \, dt_1 \\
&= \frac{1}{n!} \left(\int_{t_0}^{t} H(\tau) d\tau \right)^n \psi
\end{aligned}$$

because S_n has $n!$ elements all yielding the same contribution, the E_σ only intersect on null sets, and

$$\bigcup_{\sigma \in S_n} E_\sigma = [t_0, t]^n.$$

Figure 3.1 elucidates the argument for $n = 2$: the integration in the first two lines of (3.19) is done over a triangle whereas in the following lines we integrate over a square. The area of the triangle amounts exactly to half of the area of the square, as shown in Figure 3.1. The argument generalises to higher dimensions. Finally, (3.17) arises from the infinite sum over n.

The third case occurs when $H(t)$ is unbounded. Here, we cannot express the time evolution explicitly – at most in form of a limit – but there are theorems from the general theory of linear evolution equations establishing existence, unitarity and uniqueness of $U(t, t_0)$. In [15], Kato considers the Cauchy problem for

$$\frac{du}{dt} + A(t)u = f(t), \quad 0 \leq t \leq T, \qquad (3.20)$$

which yields the Schrödinger equation (3.15) for $A(t) = -iH(t)$ and $f \equiv 0$. We will in the following present two theorems of said work which will be employed in Chapters 4 and 5. Further results by Kato can be found in [39, 40, 41]; a related work has been contributed by Heyn [42].

Theorem 3.38. (Kato) *Let X be a Banach space and $Y \subseteq X$ a densely and continuously embedded reflexive Banach space. Let $A(t) \in \mathcal{G}(X)$ for $0 \leq t \leq T$, $T \in \mathbb{R}_0^+$, and assume that*

(i) $\{A(t)\}_{0 \leq t \leq T}$ is stable with constants M and β,

(ii) *Y is $A(t)$-admissible for each t. If $\widetilde{A}(t) \in \mathcal{G}(Y)$ is the part of $A(t)$ on Y, $\{\widetilde{A}(t)\}_{0\le t\le T}$ is stable with constants $\widetilde{M}$ and $\widetilde{\beta}$,*

(iii) *$Y \subseteq \mathcal{D}(A(t))$ such that $A(t) \in \mathcal{L}(Y,X)$ for each t and the map $t \mapsto A(t)$ is norm-continuous (Y,X).*

Then there exists a unique familiy of operators $U(t,s) \in \mathcal{L}(X)$, defined for $0 \le s \le t \le T$, such that

(a) *$U(t,s)$ is strongly continuous (X) in t, s with $U(s,s) = \mathbb{1}$ and $\|U(t,s)\|_X \le Me^{\beta(t-s)}$,*

(b) *$U(t,r) = U(t,s)U(s,r)$ for $r \le s \le t$,*

(c) *$D_t^+ U(t,s)y = -A(t)U(t,s)y$ in X for $y \in Y$, $s \le t$, and this derivative is weakly continuous (X) in t and s. $U(t,s)y$ is an indefinite integral (X) of $-A(t)U(t,s)y$ in t. In particular, $\frac{d}{dt}U(t,s)y$ exists for almost every t (depending on s) and equals $-A(t)U(t,s)y$,*

(d) *$\frac{d}{ds}U(t,s)y = U(t,s)A(s)y$ for $y \in Y$, $0 \le s \le t \le T$,*

(e) *$U(t,s)Y \subseteq Y$, $\|U(t,s)\|_Y \le \widetilde{M}e^{\widetilde{\beta}(t-s)}$ and $U(t,s)$ is weakly continuous (Y) in t and s,*

where D^+ denotes the strong right derivative (X) and $\frac{d}{ds}$ the strong derivative (X) (right derivative when $s = 0$ and left derivative when $s = t$, respectively).
The family $\{U(t,s)\}_{0\le s\le t\le T}$ is called the ***evolution operator*** *for the family $\{A(t)\}$.*

The integral in part (c) is to be understood as a Bochner integral. This is a generalisation of the concept of Lebesgue integrals to Banach space-valued functions. A rigorous definition is provided in [16, Ch. V.5].
Every Hilbert space is a reflexive Banach space, hence the theorem at hand holds in particular for Hilbert spaces Y. We will present the proof of Theorem 3.38 according to [15], Theorems 4.1 and 5.1, as it is instructive to see how the abstract operator $U(t,s)$ is constructed.
The general idea is to partition $[0,T]$ into n small intervals and to approximate the real generator $A(t)$ by a step function $A_n(t)$. On each of these small intervals, $A_n(t)$ remains constant; at the beginning of the next interval, it jumps to its new value. The finer the partition, the better is clearly the approximation, and we will show that the step function converges in some sense to the real generator as $n \to \infty$.
The time evolution $U_n(t,s)$ generated by the step function $A_n(t)$ is then constructed as follows: If s and t lie both within the same small interval where $A_n(t) \equiv A$ is constant, $U_n(t,s)$ is simply given as $\exp\{-(t-s)A\}$ by Stone's Theorem. If s and t are farer apart, $U(t,s)$ is obtained by connecting the time evolutions over all small time intervals lying in between. The exact time evolution operator $U(t,s)$ arises from this in the limit $n \to \infty$, when the step function approaches the exact generator.

Proof. Define

$$\begin{aligned} A_n : [0,T] &\longrightarrow \mathcal{G}(X) \\ t &\longmapsto A_n(t) := A\left(\tfrac{T}{n}\left[\tfrac{nt}{T}\right]\right) \end{aligned}$$

where $[r]$ denotes the largest integer which is smaller or equal r ($r \in \mathbb{R}_0^+$). A_n is constant for t varying over each interval $\left[\frac{j-1}{n}T, \frac{j}{n}T\right)$, $j = 1, \ldots, n$, respectively. Hence it is a step function with n steps, each with a width of $\frac{T}{n}$.

By assumption (iii), $t \mapsto A(t)$ is norm-continuous (Y, X), hence

$$\|A_n(t) - A(t)\|_{Y\to X} = \left\|A\left(\tfrac{T}{n}\left[\tfrac{nt}{T}\right]\right) - A(t)\right\|_{Y\to X} \xrightarrow{n\to\infty} 0 \tag{3.21}$$

uniformly in $t \in [0,T]$ as

$$\left|\tfrac{T}{n}\left[\tfrac{nt}{T}\right] - t\right| \leq \tfrac{T}{n} \xrightarrow{n\to\infty} 0.$$

$\{A_n(t)\}$ is obviously stable with the same constants M and β as $\{A(t)\}$ independent of n because the stability condition (3.13) holds by definition for *every* partition of $[0,T]$. Denoting by $\{\widetilde{A}_n\}$ the step functions approximationg $\widetilde{A}(t)$, the same is naturally true for $\{\widetilde{A}_n(t)\}$ with $\widetilde{M}, \widetilde{\beta}$.

The approximating time evolution operator $U_n(t,s)$ is defined by

$$\begin{cases} U_n(t,s) = e^{-(t-s)A} & \text{if } s,t\ (s\leq t) \text{ belong to the closure of an interval in} \\ & \text{which } A_n(t) = \mathit{const.} \equiv A, \\ U_n(t,s) = U_n(t,r)U_n(r,s) & \text{otherwise.} \end{cases}$$

It is clear that

$$\frac{d}{dt}U_n(t,s)y = -A_n(t)U_n(t,s)y \tag{3.22}$$

for $y \in Y$ and $t \neq \frac{j}{n}T$, $j \in \mathbb{N}_0$, and

$$\frac{d}{ds}U_n(t,s)y = A_n(s)U_n(t,s)y \tag{3.23}$$

for $s \neq \frac{j}{n}T$, $j \in \mathbb{N}_0$. $U_n(t,s)$ leaves Y invariant because by assumption (ii), Y is $A_n(t)$-admissible for each $t \in [0,T]$, and consequently $e^{-sA_n(t)}Y \subseteq Y$ for each $s,t \in [0,T]$. Applying Lemma 3.36, we conclude that

$$\left\|\prod_{j=1}^{k} e^{-s_j A_n(t_j)}\right\|_X \leq Me^{\beta(s_1+\cdots+s_k)}$$

for each partition $0 \leq t_1 \leq \cdots \leq t_k \leq T$, hence

$$\begin{aligned} \|U_n(t,s)\|_X &= \left\|e^{-(t-r_1)A(t)}e^{-(r_1-r_2)A(r_1)}\cdots e^{-(r_N-s)A(s)}\right\|_X \\ &\leq Me^{\beta(t-r_1+r_2-r_1+\cdots+r_N-s)} = Me^{\beta(t-s)}, \end{aligned} \tag{3.24}$$

where we have chosen $r_1, \ldots, r_N \in [0,T]$ such that $A_n(t)$ is constant on $[s, r_N], \ldots, [r_1, t]$ respectively. Analogously,

$$\|U_n(t,s)\|_Y \leq \widetilde{M}e^{\widetilde{\beta}(t-s)} \tag{3.25}$$

because $\{\widetilde{A}_n(t)\}$ is stable on Y.

In order to prove the uniform strong continuity (X) of $U_n(t,s)$ in t and s, we note that it suffices to show that

$$\operatorname*{s-lim}_{s\to 0} U_n(t,s) = U_n(t,0), \tag{3.26}$$

and analogously for t due to the semigroup property. But this is obvious: if we choose s and t so small that they lie within first small interval of the partition, we have

$$\left\|\big(U_n(t,s) - U_n(t,0)\big)x\right\|_X = \left\|e^{-(t-s)A(0)} - e^{-tA(0)}\right\|_X \xrightarrow{s\to 0} 0.$$

The convergence for arbitrary $t \in [0,T]$ follows again from the semigroup property.

Our next step is to show that the strong limit of $U_n(t,s)$ as $n\to\infty$ exists in X uniformly in t and s. We observe first that it suffices to prove that $\lim_{n\to\infty} U_n(t,s)y$ exists in X for all $y \in Y$: let $y \in Y$ and suppose $\lim_{n\to\infty} U_n(t,s)y$ exists in X. This implies that, for every $\varepsilon > 0$, there exists $N \in \mathbb{N}$ such that

$$\left\|\big(U_n(t,s) - U_m(t,s)\big)y\right\|_X < \tfrac{\varepsilon}{2} \quad \forall\, n,m \geq N.$$

Now let $x \in X$ and $\varepsilon > 0$. As Y is dense in X, we can find $y \in Y$ such that $\|x-y\|_X < \frac{\varepsilon}{4}M^{-1}e^{-\beta T}$. With (3.24) we obtain

$$\begin{aligned}\left\|\big(U_n(t,s) - U_m(t,s)\big)x\right\|_X &\leq \|(U_n(t,s) - U_m(t,s))(x-y)\|_X + \|(U_n(t,s) - U_m(t,s))y\|_X \\ &\leq 2Me^{\beta T}\,\|x-y\|_X + \|(U_n(t,s) - U_m(t,s))y\|_X < \varepsilon,\end{aligned}$$

hence $\{U_n(t,s)\}_n$ is a Cauchy sequence. As X is a Banach space, this implies

$$\operatorname*{s-lim}_{n\to\infty} U_n(t,s) = U(t,s) \in X. \tag{3.27}$$

It thus remains to show that $\lim_{n\to\infty} U_n(t,s)y$ exists in X for all $y \in Y$ uniformly in s and t. Using the fundamental theorem of calculus and (3.22) and (3.23), we express the difference between the approximating time evolution operators as

$$\begin{aligned}\big(U_n(t,r) - U_m(t,r)\big)y &= -\int_r^t \tfrac{d}{ds}\big(U_n(t,s)U_m(s,r)\big)y\,ds \\ &= -\int_r^t U_n(t,s)\big(A_n(s) - A_m(s)\big)U_m(s,r)y\,ds,\end{aligned}$$

and consequently

$$\begin{aligned}\left\|\big(U_n(t,r) - U_m(t,r)\big)y\right\|_X &\leq \int_r^t \|U_n(t,s)\|_X\,\|A_n(s) - A_m(s)\|_{Y\to X}\,\|U_m(s,r)y\|_Y\,ds \\ &\leq M\widetilde{M}e^{\gamma(t-r)}\,\|y\|_Y \int_r^t \|A_n(s) - A_m(s)\|_{Y\to X}\,ds,\end{aligned} \tag{3.28}$$

where $\gamma = \max\{\beta, \widetilde{\beta}\}$. $\|A_n(s) - A_m(s)\|_{Y\to X} \to 0$ as $n, m \to \infty$ uniformly in s by (3.21), hence we conclude the uniform existence of $U(t,s)$ in X.

We show now that $U(t,s)$ inherits properties (a) and (b) from the approximating operator $U_n(t,s)$. Assertion (b) holds by construction; the upper bound for the norm of $U(t,s)$ is an immediate consequence of (3.24). The strong continuity of $U(t,s)$ is implied by the respective property of $U_n(t,s)$ because for $x \in X$ and $\varepsilon > 0$,

$$\begin{aligned}\left\|\big(U(t,s_1) - U(t,s_2)\big)x\right\|_X \leq \left\|\big(U(t,s_1) - U_n(t,s_1)\big)x\right\|_X + \left\|\big(U_n(t,s_1) - U_n(t,s_2)\big)x\right\|_X \\ + \left\|\big(U_n(t,s_2) - U(t,s_2)\big)x\right\|_X .\end{aligned}$$

The first and third term converge to zero as $n \to \infty$ due to (3.27), and the second term becomes arbitrarily small as $s_1 \to s_2$ in consequence of the strong continuity of $U_n(t,s)$ (3.26). An analogous consideration yields sthe strong continuity in t.

Next we prove assertion (e). Let $y \in Y$. As $U_n(t,s)y$ is uniformly bounded in Y by (3.25), it contains a weakly convergent subsequence[4] in Y. We denote the weak limit by $U^{(w)}(t,s) \in Y$. On the other hand, $U_n(t,s)y$ converges to $U(t,s)y$ in X. As a consequence of both statements, $U^{(w)}(t,s)$ and $U(t,s)$ must coincide, and we conclude that $U(t,s)y \in Y$. This being established, the upper bound for $\|U(t,s)\|_Y$ follows from (3.25).
The weak continuity (Y) of $U(t,s)$ can be shown as follows: Let $t_j \to t_0$ and $s_j \to s_0$. By the same argument as above, any subsequence of $\{U(t_j,s_j)y\}$ contains a subsequence that converges weakly in Y towards the limit $U^{(w)}(t_0,s_0)y = U(t_0,s_0)$. Hence $U(t,s)$ is weakly continuous in Y.

Before proceeding to assertions (c) and (d), we introduce the following lemma:

Lemma 3.39. *Let $\{A'(t)\}_{0\leq t\leq T}$ be another family satisfying the assumptions of Theorem 3.38 with the same X and Y and with the constants of stability M', β', $\widetilde{M}'$ and $\widetilde{\beta}'$. Let $\{U'(t,s)\}_{0\leq s\leq t\leq T}$ be constructed from $\{A'(t)\}_{0\leq t\leq T}$ in the same way as $\{U(t,s)\}$ was constructed above from $\{A(t)\}$. Then*

$$\left\|\big(U'(t,r) - U(t,r)\big)y\right\|_X \leq M'\widetilde{M}e^{\gamma(t-r)}\,\|y\|_Y \int_r^t \left\|A'(s) - A(s)\right\|_{Y\to X} ds, \tag{3.29}$$

where $\gamma = \max\{\beta', \widetilde{\beta}\}$.

Proof. One estimates the norm analogously to (3.28) and takes the limit $n \to \infty$. □

To show (c) and (d), we fix first $r \in [0,T]$ and put $A'(s) = A(r) = const.$ for $s \in [0,T]$. Due to the mean value theorem for integrals[5] there exists $\xi \in [r,t]$ such that

$$\int_r^t \|A(s)\|_{Y\to X}\, ds = \|A(\xi)\|_{Y\to X}\,(t-r)$$

[4] See e.g. [43], Theorem III.3.7.
[5] See e.g. [44, Ch. 11.3]

as $t \mapsto \|A(t)\|_{Y\to X}$ is continuous. Hence the right hand side of (3.29) is of order

$$M'\widetilde{M}e^{\gamma(t-r)}\,\|y\|_Y \int_r^t \big\|A'(s) - A(s)\big\|_{Y\to X}\,ds \sim \mathcal{O}(t-r) \tag{3.30}$$

as $t \searrow r$. On the left hand side of (3.29) we have $U'(t,r) = e^{-(t-r)A(r)}$, whose right derivative is given by

$$D_t^+ U'(t,r)y\big|_{t=r} = -A(r)y. \tag{3.31}$$

(3.30) implies that the difference $\|(U'(t,r) - U(t,r))y\|_X$ is at most of order $\mathcal{O}(t-r)$, and together with (3.31) we conclude

$$D_t^+ U(t,s)y\big|_{t=s} = -A(s)y, \tag{3.32}$$

because $U(t,s)y|_{t=s} = U'(t,s)y|_{t=s}$ by construction and the first derivative is precisely the approximation of a function to first order.
We now fix t instead of r and put $A'(s) = A(t) = const.$ for $s \in [0,T]$. An analogous reasoning yields

$$D_s^- U(t,s)y\big|_{t=s} = A(t)y. \tag{3.33}$$

For $s < t$, we obtain

$$\begin{aligned} D_s^+ U(t,s)y &= \lim_{h\downarrow 0}\left[\tfrac{1}{h}\big(U(t,s+h)y - U(t,s)y\big)\right] \\ &= \lim_{h\downarrow 0}\left[U(t,s+h)\tfrac{1}{h}\big(y - U(s+h,s)y\big)\right], \end{aligned}$$

and by (3.32) and the strong continuity of $U(t,s)$ we conclude

$$D_s^+ U(t,s)y = U(t,s)A(s)y. \tag{3.34}$$

For $s \le t$, one computes analogously

$$\begin{aligned} D_s^- U(t,s)y &= \lim_{h\downarrow 0}\left[\tfrac{1}{h}\big(U(t,s)y - U(t,s-h)y\big)\right] \\ &= U(t,s)\; D_s^- U'(t,s)y\big|_{t=s}, \end{aligned}$$

hence we conclude from (3.33) that

$$D_s^- U(t,s)y = U(t,s)A(s)y. \tag{3.35}$$

As the right derivative (3.34) and the left derivative (3.35) agree for all $s,t \in [0,T]$, assertion (d) follows. To show (c), we compute for $s \le t$

$$\begin{aligned} D_t^+ U(t,s)y &= \lim_{h\downarrow 0}\left[\tfrac{1}{h}\big(U(t+h,s)y - U(t,s)y\big)\right] \\ &= \lim_{h\downarrow 0}\left[\tfrac{1}{h}\big(\mathbb{1} - U(t,t+h)\big)U(t+h,s)y\right]. \end{aligned}$$

By (e), $U(t+h,s)y \in Y$, and consequently (3.34) implies

$$D_t^+ U(t,s)y = -A(t)U(t,s)y. \tag{3.36}$$

The right derivative $D_t^+ U(t,s)y$ is weakly continuous (X) because $U(t,s)$ is weakly continuous (Y) and $A(t)$ is norm-continuous (Y,X). Hence $-A(t)U(t,s)$ is measurable, which proves the last part of (c).

At last we show that the hereby constructed time evolution operator $U(t,s)$ is unique. Let $\{V(t,s)\}_{0\le s\le t\le T}$ be another family satisfying (a) and (d). Then (3.22) and (d) imply

$$\big(V(t,r) - U_n(t,r)\big)y = -\int_r^t V(t,s)\big(A(s) - A_n(s)\big)U_n(s,r)y\,ds$$

for every $y \in Y$, and consequently

$$\begin{aligned}\|(V(t,r) - U_n(t,r))y\|_X &\le \int_t^r \|V(t,s)\|_X \,\|A(s) - A_n(s)\|_{Y\to X}\,\|U_n(s,r)y\|_Y\,ds \\ &\le M\widetilde{M}e^{\gamma(t-r)}\,\|y\|_Y \int_t^r \|A(s) - A_n(s)\|_{Y\to X}\,ds,\end{aligned}$$

where as above $\gamma = \max\{\beta, \widetilde{\beta}\}$. This expression converges to zero as $n \to \infty$ by (3.21), hence $V(t,r) = U(t,r)$. □

When applying Theorem 3.38 to concrete situations, it is sometimes difficult to verify condition (ii). The following lemma gives a criterion that is sufficient for (ii) to hold, and might be easier to prove. In fact, we will use precisely this condition in Section 4.2.3.

Lemma 3.40. *Condition (ii) in Theorem 3.38 is implied by*

(ii') There is a family $\{S(t)\}_{0\le t\le T}$ of isomorphisms of Y onto X such that
- *(1) $S(t)A(t)S(t)^{-1} = A_1(t) \in \mathcal{G}(X)$ for $0 \le t \le T$,*
- *(2) $\{A_1(t)\}_{0\le t\le T}$ is a stable family with constants M_1 and β_1,*
- *(3) there is a constant $\gamma \in \mathbb{R}$ such that $\|S(t)\|_{Y\to X} \le \gamma$ and $\left\|S(t)^{-1}\right\|_{X\to Y} \le \gamma$,*
- *(4) $\{S(t)\}_{0\le t\le T}$ is of bounded variation with respect to $\|\cdot\|_{Y\to X}$.*

In particular, $\{\widetilde{A}(t)\}$ is stable with constants $\widetilde{M} = M_1\gamma^2 e^{\gamma M_1 V}$ and $\widetilde{\beta} = \beta_1$, where V denotes the total variation of $S(t)$.

Proof. [15, Proposition 4.4]. According to Lemma 3.34, (ii') implies that Y is $A(t)$-admissible. Let $\widetilde{A}(t) \in \mathcal{G}(Y)$ be the part of $A(t)$ on Y. By definition,

$$\mathcal{D}(A_1(t)) = \mathcal{D}\big(S(t)A(t)S(t)^{-1}\big) = \{x \in X : S(t)^{-1}x \in \mathcal{D}(A(t)),\ A(t)S(t)^{-1}x \in Y\}.$$

Hence $A_1(t) + \lambda = S(t)(A(t)+\lambda)^{-1}S(t)^{-1}$ for any λ, and consequently

$$(\widetilde{A}(t)+\lambda)^{-1} = S(t)^{-1}(A_1(t)+\lambda)^{-1}S(t),$$

which leads to

$$\prod_{j=1}^{k} R_\lambda(-\widetilde{A}(t_j)) = \prod_{j=1}^{k} S(t_j)^{-1} R_\lambda(-A_1(t_j)) S(t_j). \tag{3.37}$$

With

$$P_j := \big(S(t_j) - S(t_{j-1})\big) S(t_{j-1})^{-1} = S(t_j) S(t_{j-1})^{-1} - \mathbb{1},$$

we can express (3.37) as

$$S(t_k)^{-1} \Big[R_\lambda(-A_1(t_k))(\mathbb{1} + P_k) R_\lambda(-A_1(t_{k-1})) \cdots (\mathbb{1} + P_2) R_\lambda(-A_1(t_1)) \Big] S(t_1). \tag{3.38}$$

The X-norm of the expression within the brackets in (3.38) has the upper bound

$$\begin{aligned}
&\| R_\lambda(-A_1(t_k)) P_k R_\lambda(-A_1(t_{k-1})) P_{k-1} \cdots P_2 R_\lambda(-A_1(t_1)) \|_X \\
&\quad + \sum_{j=2}^{k} \Big\| R_\lambda(-A_1(t_k)) P_k \cdots \breve{P}_j \cdots P_2 R_\lambda(-A_1(t_1)) \Big\|_X \\
&\quad + \sum_{\substack{j_1, j_2 = 2 \\ j_1 \neq j_2}}^{k} \Big\| R_\lambda(-A_1(t_k)) P_k \cdots \breve{P}_{j_1} \cdots \breve{P}_{j_2} \cdots P_2 R_\lambda(-A_1(t_1)) \Big\|_X \\
&\quad + \ldots \\
&\quad + \| R_\lambda(-A_1(t_k)) \cdots R_\lambda(-A_1(t_1)) \|_X ,
\end{aligned}$$

where $\breve{P}_j$ signifies that this factor of the product is left out. Since $\{A_1(t)\}$ is stable, this is bounded above by

$$\begin{aligned}
(\lambda - \beta_1)^{-k} \Bigg[& M_1^k \|P_k\|_X \cdots \|P_2\|_X + M_1^{k-1} \sum_{j=2}^{k} \|P_k\|_X \cdots \big\|\breve{P}_j\big\|_X \cdots \|P_2\|_X + \ldots \\
& + M_1 \sum_{j=2}^{k} \|P_j\|_X + M_1 \Bigg]
\end{aligned}$$

according to Definition 3.35. It can easily be verified that this equals

$$M_1 (\lambda - \beta_1)^{-k} (1 + M_1 \|P_k\|_X) \cdots (1 + M_1 \|P_2\|_X). \tag{3.39}$$

We recall that $\|P_j\|_X \leq \gamma \|S(t_j) - S(t_{j-1})\|_{Y \to X}$ by assumption and that $S(t)$ is of bounded variation (Y, X). Due to (3.39), the X-norm of (3.37) has the upper bound

$$\begin{aligned}
& M_1 \gamma^2 \left(1 + \gamma M_1 \|S(t_k) - S(t_{k-1})\|_{Y \to X}\right) \cdots \left(1 + \gamma M_1 \|S(t_2) - S(t_1)\|_{Y \to X}\right) (\lambda - \beta_1)^{-k} \\
&\quad \leq M_1 \gamma^2 \exp\left\{ \gamma M_1 \|S(t_k) - S(t_{k-1})\|_{Y \to X} \right\} \cdots \exp\left\{ \gamma M_1 \|S(t_2) - S(t_1)\|_{Y \to X} \right\} (\lambda - \beta_1)^{-k} \\
&\quad \leq M_1 \gamma^2 e^{\gamma M_1 V} (\lambda - \beta_1)^{-k},
\end{aligned}$$

where V denotes the total variation of $S(t)$ as in Definition 3.1. Hence we have shown that $\{\widetilde{A}(t)\}$ is stable with constants $\widetilde{M} = M_1 \gamma^2 e^{\gamma M_1 V}$ and $\widetilde{\beta} = \beta_1$. □

Finally, we replace condition (ii) by a more abstract condition. This enables us to drop the requirement of Y being reflexive, and besides to expand the assertions of Theorem 3.38 by two new statements.

Theorem 3.41. *Let X, Y be Banach spaces, $Y \subseteq X$ densely and continuously embedded and $A(t) \in \mathcal{G}(X)$ for $0 \leq t \leq T$, $T \in \mathbb{R}_0^+$. Assume (i) and (iii) of Theorem 3.38 and replace (ii) by*

(ii") There is a family $\{S(t)\}_{0 \leq t \leq T}$ of isomorphisms of Y onto X such that

- *(1) $t \mapsto S(t)$ is continuously differentiable (Y, X),*
- *(2) $S(t)A(t)S(t)^{-1} = A(t) + B(t)$ where $B(t) \in \mathcal{L}(X)$,*
- *(3) $t \mapsto B(t)$ is strongly continuous (X).*

Then conclusions (a) to (e) of Theorem 3.38 are true. Further,

- *(f) $U(t, s)$ is strongly continuous (Y) jointly in t and s,*
- *(g) for each fixed $y \in Y$ and $s \in [0, T]$, $\frac{d}{dt}U(t, s)y$ exists for all $t \geq s$, equals $-A(t)U(t, s)y$ and is strongly continuous (X) in t.*

The complete proof can be found in [15] (Theorems 5.2 and 6.1). We will in the sequel briefly present the main ideas of the argument.

Outline of the proof. One shows first that assumption (ii") implies (ii') with $A_1(t) = A(t) + B(t)$. This follows because the stability of $\{A(t)\}$ implies the stability of $A(t) + B(t)$ for uniformly bounded $B(t)$ (Proposition 3.5 in [15]). $S(t)$ and $S(t)^{-1}$ are both norm-Lipschitz continuous (X, Y) and hence of bounded variation.
The generalisation from Y being a Hilbert space to it being a mere Banach space only affects the proof of assertion (e) in Theorem 3.38, where we have used that the bounded sequence $U_n(t, s)$ has a weakly convergent subsequence in the Hilbert space Y. This also concerns assertion (c), which builds upon (e).
Instead of using the reflexivity of Y, one shows now that $W(t, s) := S(t)U(t, s)S(s)^{-1}$ belongs to $\mathcal{L}(X)$ and is strongly continuous (X) jointly in s and t. We refrain from expanding on this step here – it works analogously to the respective part of the proof of the following Theorem 3.42, which we will discuss in detail.
These properties of $W(t, s)$ being established, assertion (e) follows because for $y \in Y$,

$$\|U(t, s)y\| = \left\|S(t)^{-1}W(t, s)S(s)y\right\|_Y \leq \gamma^2 \|W(t, s)\|_X \|y\|_Y ,$$

where γ is the common upper bound of $S(t)^{-1}$ and $S(t)$ from condition (ii'). Hence $U(t, s)Y \subseteq Y$ and $U(t, s)$ is strongly and thus weakly continuous (Y) in s, t.
The joint strong continuity (Y) of $U(t, s)$ claimed in (f) is obvious because for $y \in Y$,

$$\begin{aligned}\left\|\big(U(t_1, s_1) - U(t_2, s_2)\big)y\right\|_Y &= \left\|\big(S(t_1)^{-1}W(t_1, s_1)S(s_1) - S(t_2)^{-1}W(t_2, s_2)S(s_2)\big)y\right\|_Y \\ &\leq \gamma^2 \|W(t_1, s_1) - W(t_2, s_2)\|_X \|y\|_Y\end{aligned}$$

and $W(t, s)$ is jointly strongly continuous. Further, $A(t)U(t, s)y$ is continuous (X) in t, which together with (c) proves (g). $\square$

A result very similar to KATO's theorems, but under different assumptions[6], has been achieved by YOSIDA [16]. The author constructs the solution of the Cauchy problem

$$\frac{dx(t)}{dt} = A(t)x(t); \quad x(s) = y \tag{3.40}$$

and proves several properties of the time evolution operator. Note that as opposed to (3.20), the generator $A(t)$ of the evolution in (3.40) exhibits the opposite sign.

Theorem 3.42. (YOSIDA) *Let X be a Banach space and $A(t) : X \supseteq \mathcal{D}(A(t)) \to X$ for $t \in [0,T]$. For any $n \in \mathbb{N}$ and $0 \leq s \leq t \leq T$ define $U_n(s,t) \in \mathcal{L}(X)$ by*

$$\begin{cases} U_n(t,s) = e^{(t-s)A\left(\frac{j-1}{n}T\right)} & \text{if} \quad \frac{j-1}{n}T \leq s \leq t \leq \frac{j}{n}T \quad \text{for} \ 1 \leq j \leq n \\ U_n(t,s) = U_n(t,r)U_n(r,s) & \text{if} \quad 0 \leq s \leq r \leq t \leq T\,. \end{cases}$$

Assume that

(i) $\mathcal{D}(A(t)) \equiv \mathcal{D}$ is independent of t and dense in X,

(ii) $R_\lambda(A(t)) \in \mathcal{L}(X)$ for every $\lambda \geq 0$, $t \in [0,T]$, such that $\|R_\lambda(A(t))\|_X \leq \frac{1}{\lambda}$ for $\lambda > 0$,

(iii) $A(t)A(s)^{-1} \in \mathcal{L}(X)$ for $s,t \in [0,T]$,

(iv) Define $C(t,s) := A(t)A(s)^{-1} - \mathbb{1}$. For each $x \in X$,

(1) $(s,t) \mapsto \frac{1}{t-s}C(t,s)x$ is bounded and uniformly continuous in t and s, $t \neq s$,

(2) $C(t)x := \lim_{n\to\infty} nC(t,t-\frac{1}{n})x$ exists uniformly in t,

(3) $t \mapsto C(t)x$ is norm-continuous.

Then it holds for every $x \in X$ and $0 \leq s \leq t \leq T$ that

(a) $\lim_{n\to\infty} U_n(t,s)x = U(t,s)x$ exists uniformly in t and s,

(b) for $y \in \mathcal{D}$, the Cauchy problem

$$\frac{dx(t)}{dt} = A(t)x(t), \quad x(s) = y, \quad x(t) \in \mathcal{D}$$

is solved by $x(t) = U(t,s)y$ with $\|x(t)\|_X \leq \|y\|_X$,

(c) $U(t,s)$ is uniformly strongly continuous jointly in t and s,

(d) $U(t,s)$ leaves $\mathcal{D}$ invariant.

The construction of $U(t,s)$ is exactly the same as in Theorem 3.38. For $n \in \mathbb{N}$, the approximating time evolution $U_n(t,s)$ equals

$$\begin{aligned} U_n(t,s) &= U_n\big(t, \tfrac{T}{n}\left[\tfrac{nt}{T}\right]\big)U_n\big(\tfrac{T}{n}\left[\tfrac{nt}{T}\right], \tfrac{T}{n}\left(\left[\tfrac{nt}{T}\right]-1\right)\big)\cdots U_n\left(\tfrac{T}{n}\left(\left[\tfrac{ns}{T}\right]+1\right), s\right) \\ &= e^{\left(t-\frac{T}{n}\left[\frac{nt}{T}\right]\right)A\left(\frac{T}{n}\left[\frac{nt}{T}\right]\right)} \cdots e^{\left(\frac{T}{n}\left(\left[\frac{ns}{T}\right]+1\right)-s\right)A\left(\frac{T}{n}\left[\frac{ns}{T}\right]\right)}. \end{aligned} \tag{3.41}$$

[6] YOSIDA's assumptions are in fact equivalent to the assumptions KATO makes in [39]. A rigorous proof of this statement is given in [36].

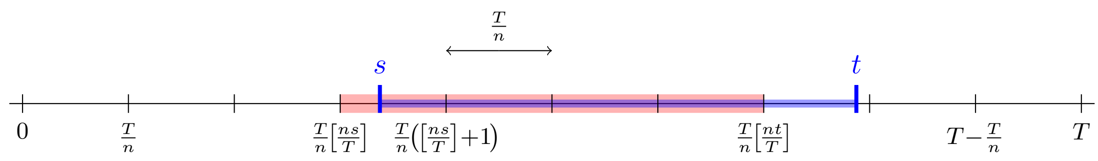

Figure 3.2: Partitioning of $[0,T]$ into $n = 10$ small subintervals. The interval $[s,t]$ is highlighted in blue, the intervals contributing to $m_n(t,s)$ are marked red.

The construction is easier to grasp for $T = 1$: in this case, (3.41) can be written more compactly as

$$\begin{aligned} U_n(t,s) &= U_n\left(t, \tfrac{[nt]}{n}\right) U_n\left(\tfrac{[nt]}{n}, \tfrac{[nt]-1}{n}\right) \cdots U_n\left(\tfrac{[ns]+1}{n}, s\right) \\ &= e^{\left(t-\frac{[nt]}{n}\right)A\left(\frac{[nt]}{n}\right)} \cdots e^{\left(\frac{[ns]+1}{n}-s\right)A\left(\frac{[ns]}{n}\right)}. \end{aligned} \tag{3.42}$$

Note that not all intervals are of equal length. As can be seen in Figure 3.2, the length of the first and the last interval, $\left[s, \frac{T}{n}\left(\left[\frac{ns}{T}\right]+1\right)\right)$ and $\left[\frac{T}{n}\left[\frac{nt}{T}\right], t\right)$, may be smaller or equal $\frac{T}{n}$ whereas all intervals in between have a length of exactly $\frac{T}{n}$.

We present a proof of this theorem which is taken from [16, Ch. XIV], Theorem 1, [14], Theorem X.70, and [35], Lemma 3.12. We adapt the proof in such a way that T may be any non-negative finite number and is not confined to the case $T = 1$.

Proof. Define

$$W_n(t,s) = A(t)U_n(t,s)A(s)^{-1}. \tag{3.43}$$

Our first step is to provide an estimate for $\|W_n(t,s)x\|_X$, $x \in X$. We abbreviate $\|\cdot\|_X$ by $\|\cdot\|$. Then

$$\begin{aligned} W_n(t,s) = A(t)e^{\left(t-\frac{T}{n}\left[\frac{nt}{T}\right]\right)A\left(\frac{T}{n}\left[\frac{nt}{T}\right]\right)} A\left(\tfrac{T}{n}\left[\tfrac{nt}{T}\right]\right)^{-1} A\left(\tfrac{T}{n}\left[\tfrac{nt}{T}\right]\right) \cdots \cdot \\ \cdot\ e^{\left(\frac{T}{n}\left(\left[\frac{ns}{T}\right]+1\right)-s\right)A\left(\frac{T}{n}\left[\frac{ns}{T}\right]\right)} A\left(\tfrac{T}{n}\left[\tfrac{ns}{T}\right]\right)^{-1} A\left(\tfrac{T}{n}\left[\tfrac{ns}{T}\right]\right) A(s)^{-1}. \end{aligned} \tag{3.44}$$

Using the fact that a semigroup commutes with its generator (Theorem 3.29) and the definition

$$C(t,s) = A(t)A(s)^{-1} - \mathbb{1}$$

from assumption (iv), we can rewrite (3.44) as

$$\begin{aligned} W_n(t,s) = \Big(\mathbb{1} + C\left(t, \tfrac{T}{n}\left[\tfrac{nt}{T}\right]\right)\Big) \Big[& U_n\left(t, \tfrac{T}{n}\left[\tfrac{nt}{T}\right]\right) \Big(\mathbb{1} + C\left(\tfrac{T}{n}\left[\tfrac{nt}{T}\right], \tfrac{T}{n}\left(\left[\tfrac{nt}{T}\right]-1\right)\right)\Big) \cdot \\ & \cdot U_n\left(\tfrac{T}{n}\left[\tfrac{nt}{T}\right], \tfrac{T}{n}\left(\left[\tfrac{nt}{T}\right]-1\right)\right) \cdots \cdot \\ & \cdot U_n\left(\tfrac{T}{n}\left(\left[\tfrac{ns}{T}\right]+1\right), s\right) \Big] \Big(\mathbb{1} + C\left(\tfrac{T}{n}\left[\tfrac{ns}{T}\right], s\right)\Big). \end{aligned} \tag{3.45}$$

Expanding the product within the square brackets in (3.45) yields

$$W_n(t,s) = \left(\mathbb{1} + C\left(t, \tfrac{T}{n}\left[\tfrac{nt}{T}\right]\right)\right)\Bigg[U_n(t,s) + \sum_{u=\left[\frac{ns}{T}\right]+1}^{\left[\frac{nt}{T}\right]} U_n\left(t, \tfrac{Tu}{n}\right) C\left(\tfrac{Tu}{n}, \tfrac{T(u-1)}{n}\right) U_n\left(\tfrac{Tu}{n}, s\right) + \dots\Bigg]\left(\mathbb{1} + C\left(\tfrac{T}{n}\left[\tfrac{ns}{T}\right]\right), s\right), \tag{3.46}$$

where we have grouped together those terms of the expansion which contain equal numbers of $C(t,s)$, respectively. Introducing the notation

$$\begin{aligned}
W_n^{(0)}(t,s) &= U_n(t,s),\\
W_n^{(1)}(t,s) &= \sum_{u=\left[\frac{ns}{T}\right]+1}^{\left[\frac{nt}{T}\right]} U_n\left(t, \tfrac{Tu}{n}\right) C\left(\tfrac{Tu}{n}, \tfrac{T(u-1)}{n}\right) U_n\left(\tfrac{Tu}{n}, s\right),\\
&\dots\\
W_n^{(m)}(t,s) &= \sum_{u_1=\left[\frac{ns}{T}\right]+m}^{\left[\frac{nt}{T}\right]} \cdots \sum_{u_m=\left[\frac{ns}{T}\right]+1}^{u_{m-1}-1} U_n\left(t, \tfrac{Tu_1}{n}\right) C\left(\tfrac{Tu_1}{n}, \tfrac{T(u_1-1)}{n}\right) U_n\left(\tfrac{Tu_1}{n}, \tfrac{Tu_2}{n}\right) \cdot\\
&\quad \cdot C\left(\tfrac{Tu_2}{n}, \tfrac{T(u_2-1)}{n}\right) \cdots U_n\left(\tfrac{Tu_{m-1}}{n}, \tfrac{Tu_m}{n}\right) C\left(\tfrac{Tu_m}{n}, \tfrac{T(u_m-1)}{n}\right) U_n\left(\tfrac{Tu_m}{n}, s\right),
\end{aligned}$$

we write (3.46) as

$$\begin{aligned}
W_n(t,s) = \left(\mathbb{1} + C\left(t, \tfrac{T}{n}\left[\tfrac{nt}{T}\right]\right)\right)\left[W_n^{(0)}(t,s) + W_n^{(1)}(t,s) + \dots + W_n^{(m_n(t,s))}(t,s)\right] \cdot\\
\cdot \left(\mathbb{1} + C\left(\tfrac{T}{n}\left[\tfrac{ns}{T}\right]\right), s\right),
\end{aligned} \tag{3.47}$$

where

$$m_n(t,s) = \max\left\{m \in \mathbb{N} : \left[\tfrac{ns}{T}\right] + m \leq \left[\tfrac{nt}{T}\right]\right\} \in \mathbb{N}_0. \tag{3.48}$$

As shown in Figure 3.2, $m_n(t,s)$ is the number of intervals between $\left[\frac{ns}{T}\right]$ and $\left[\frac{nt}{T}\right]$, hence $m_n(t,s)+1$ is the number of factors in (3.41). Define

$$N := \sup_{\substack{s,t \in [0,T]\\ s \neq t}} \left\| \tfrac{1}{t-s} C(t,s) \right\|, \tag{3.49}$$

which is finite by assumption (iv). We note that

$$\|U_n(t,s)\| \leq 1, \tag{3.50}$$

as assumptions (i) and (ii) imply by the HILLE-YOSIDA theorem that $A(s)$ is the generator of the contraction semigroup $\{e^{tA(s)}\}_{t\geq 0}$. With (3.49) and (3.50), we estimate the norm of

$W_n^{(m)}(t,s)$ as

$$\begin{aligned}\left\|W_n^{(m)}(t,s)\right\| &\le \sum_{u_1=\left[\frac{ns}{T}\right]+m}^{\left[\frac{nt}{T}\right]} \cdots \sum_{u_m=\left[\frac{ns}{T}\right]+1}^{u_{m-1}-1} \left\|C\left(\tfrac{Tu_1}{n}, \tfrac{T(u_1-1)}{n}\right)\right\| \cdots \left\|C\left(\tfrac{Tu_m}{n}, \tfrac{T(u_m-1)}{n}\right)\right\| \\ &\le \left(\tfrac{NT}{n}\right)^m \sum_{u_1=\left[\frac{ns}{T}\right]+m}^{\left[\frac{nt}{T}\right]} \cdots \sum_{u_m=\left[\frac{ns}{T}\right]+1}^{u_{m-1}-1} 1.\end{aligned}$$

Analogously to the argument in (3.19), we bring the sums into a form where $u_1,\ldots,u_m$ vary over the same region $\left[\left[\frac{ns}{T}\right]+1, \left[\frac{nt}{T}\right]\right]$. As shown in Figure 3.1, we morally change the domain of summation from a triangle to a square (or their higher-dimensional analogues, respectively), which yields a factor $\frac{1}{m!}$. Thus

$$\left\|W_n^{(m)}(t,s)\right\| \le \left(\frac{NT}{n}\right)^m \frac{\left(\left[\frac{nt}{T}\right] - \left(\left[\frac{ns}{T}\right]+1\right)\right)^m}{m!} \le \frac{(N(t-s))^m}{m!}, \tag{3.51}$$

where we have used that $[kt]-[ks] \le k(t-s)+1$ for $k>0$. Hence the desired estimate for $W_n(t,s)$ is given by

$$\|W_n(t,s)\| \le \left(1+\tfrac{TN}{n}\right)^2 e^{N(t-s)} \le \left(1+\tfrac{TN}{n}\right)^2 e^{NT}. \tag{3.52}$$

Our next task is to establish the convergence $U_n(t,s) \to U(t,s)$ in the limit $n\to\infty$. Similarly to the proof of Kato's theorem, we will express the difference between $U_n(t,s)$ and $U_k(t,s)$ by the difference of their generators and thus show that $\{U_n(t,s)\}_{n\in\mathbb{N}}$ is a Cauchy sequence. To this end, we need to compute the derivatives in t and s of the approximating operators $U_n(t,s)$.

We note first that $U_n(t,s)$ leaves $\mathcal{D}$ invariant because for $y\in\mathcal{D}(A(s))\equiv\mathcal{D}$,

$$\|A(t)U_n(t,s)y\| = \|W_n(t,s)A(s)y\| \le \left(1+\tfrac{TN}{n}\right)^2 e^{N(t-s)}\,\|A(s)y\| \tag{3.53}$$

by (3.52), which is finite as $y\in\mathcal{D}$. Consequently, $U_n(t,s)y\in\mathcal{D}(A(t))\equiv\mathcal{D}$. This implies that $U_n(t,s)y$ is differentiable at $t\neq\frac{j}{n}$ and at $s\neq\frac{j}{n}$, $j=0,\ldots,n$. The derivatives can be calculated as

$$\begin{aligned}\tfrac{d}{dt}U_n(t,s)y &= \tfrac{d}{dt}e^{\left(t-\frac{T}{n}\left[\frac{nt}{T}\right]\right)A\left(\frac{T}{n}\left[\frac{nt}{T}\right]\right)}U_n\left(\tfrac{T}{n}\left[\tfrac{nt}{T}\right],s\right)y \\ &= A\left(\tfrac{T}{n}\left[\tfrac{nt}{T}\right]\right)U_n(t,s)y\end{aligned} \tag{3.54}$$

and

$$\begin{aligned}\tfrac{d}{ds}U_n(t,s)y &= \tfrac{d}{ds}U_n\left(t,\tfrac{T}{n}\left(\left[\tfrac{ns}{T}\right]+1\right)\right)e^{\left(\frac{T}{n}\left(\left[\frac{ns}{T}\right]+1\right)-s\right)A\left(\frac{T}{n}\left[\frac{ns}{T}\right]\right)}y \\ &= -U_n(t,s)A\left(\tfrac{T}{n}\left[\tfrac{ns}{T}\right]\right)y\end{aligned} \tag{3.55}$$

for $y\in\mathcal{D}$ in both cases. Taking $x=A(0)y$, we see that for every y, the t-derivative (3.54) is bounded, except at $t=\frac{j}{k}$, $j=0,1,\ldots,n$, because

$$\begin{aligned}\tfrac{d}{dt}U_n(t,s)y &= A\left(\tfrac{T}{n}\left[\tfrac{nt}{T}\right]\right)A(t)^{-1}A(t)U_n(t,s)A(s)^{-1}A(s)A(0)^{-1}x \\ &= \left(\mathbb{1}+C\left(\tfrac{T}{n}\left[\tfrac{nt}{T}\right],t\right)\right)W_n(t,s)\left(\mathbb{1}+C(s,0)\right)x,\end{aligned} \tag{3.56}$$

and consequently

$$\left\|\tfrac{d}{dt}U_n(t,s)y\right\| \leq \left(1+\left\|C\left(\tfrac{T}{n}\left[\tfrac{nt}{T}\right],t\right)\right\|\right)\left(1+\|C(s,0)\|\right)\|W_n(t,s)\|\,. \tag{3.57}$$

This is bounded uniformly in t and s by (3.49) and (3.52). As $C(t,s)$ is strongly continuous by assumption (iv), $U_n(t,s)y$ is moreover strongly continuous in t and s, except at $t=\frac{j}{k}$, $j=0,1,\dots,n$.
Analogously, we find that the s-derivative (3.55) is also bounded and strongly continuous in t and s, except at $s=\frac{j}{k}$, $j=0,1,\dots,n$, due to

$$\begin{aligned}\left\|\tfrac{d}{ds}U_n(t,s)y\right\| &\leq \|U_n(t,s)\|\left\|A\left(\tfrac{T}{n}\left[\tfrac{ns}{T}\right]\right)A(0)^{-1}\right\|\|x\|\\ &\leq \left(1+\left\|C\left(\tfrac{T}{n}\left[\tfrac{ns}{T}\right],0\right)\right\|\right)\|x\|\end{aligned} \tag{3.58}$$

as a consequence of (3.50).
We show now that $\{U_n(t,s)x\}_{n\in\mathbb{N}}$ is a Cauchy sequence for every $x\in X$. Let $n,k\in\mathbb{N}_0$. Then

$$\begin{aligned}&\big(U_k(t,s)-U_n(t,s)\big)A(0)^{-1}x\\ &\quad=\int_s^t \tfrac{d}{dr}\big(U_n(t,r)U_k(r,s)A(0)^{-1}x\big)dr\\ &\quad=\int_s^t U_n(t,r)\Big[A\left(\tfrac{T}{k}\left[\tfrac{kr}{T}\right]\right)-A\left(\tfrac{T}{n}\left[\tfrac{nr}{T}\right]\right)\Big]A\left(\tfrac{T}{k}\left[\tfrac{kr}{T}\right]\right)^{-1}A\left(\tfrac{T}{k}\left[\tfrac{kr}{T}\right]\right)U_k(r,s)A(0)^{-1}x\,dr\\ &\quad=-\int_s^t U_n(t,r)C\left(\tfrac{T}{n}\left[\tfrac{nr}{T}\right],\tfrac{T}{k}\left[\tfrac{kr}{T}\right]\right)\Big(\mathbb{1}+C\left(\tfrac{T}{k}\left[\tfrac{kr}{T}\right],r\right)\Big)W_k(r,s)\Big(\mathbb{1}+C(s,0)\Big)x\,dr,\end{aligned}$$

hence

$$\begin{aligned}&\left\|\big(U_k(t,s)-U_n(t,s)\big)A(0)^{-1}x\right\|\\ &\quad\leq N(1+sN)\left(1+\tfrac{TN}{n}\right)^2\int_s^t\left|\tfrac{T}{n}\left[\tfrac{nr}{T}\right]-\tfrac{T}{k}\left[\tfrac{kr}{T}\right]\right|\Big(1+N\left(r-\tfrac{T}{k}\left[\tfrac{kr}{T}\right]\right)\Big)e^{N(r-s)}\|x\|\,dr\\ &\quad\leq N(1+TN)e^{NT}\|x\|\int_s^t\left|\tfrac{T}{n}\left[\tfrac{nr}{T}\right]-\tfrac{T}{k}\left[\tfrac{kr}{T}\right]\right|\left(1+\tfrac{NT}{k}\right)\left(1+\tfrac{TN}{n}\right)^2dr,\end{aligned}$$

which converges to zero when $n,k\to\infty$. Thus $\{U_n(t,s)\}_{n\in\mathbb{N}}$ is a Cauchy sequence and due to the completeness of X, $\lim_{n\to\infty}U_n(t,s)A(0)^{-1}x$ exists uniformly in t and s. As $\mathcal{D}\equiv\mathcal{D}(A(0))$ is dense in X and $U_n(t,s)$ is uniformly bounded by (3.50), we conclude that $\lim_{n\to\infty}U_n(t,s)x$ exists for every $x\in X$ uniformly in t and s. This proves assertion (a).

It is clear that $\|U(t,s)\|\leq 1$ and $U(t,s)U(s,r)=U(t,r)$ for $r,s,t\in[0,T]$. We deduce further that $U(t,s)$ is uniformly strongly continuous jointly in t and s: Let $(t,s)\to(t_0,s_0)$ and assume without loss of generality that $t\leq t_0$. Then

$$\begin{aligned}\|U(t,s)-U(t_0,s_0)\| &\leq \|U(t,s)-U_n(t,s)\|+\|U_n(t,s)-U_n(t_0,s)\|\\ &\quad+\|U_n(t_0,s)-U_n(t_0,s_0)\|+\|U_n(t_0,s_0)-U(t_0,s_0)\|\,.\end{aligned} \tag{3.59}$$

The first and the last term converge to zero by (a). As $t \searrow t_0$, t eventually ends up within the interval $\left[\frac{T}{n}\left[\frac{nt_0}{T}\right], t_0\right]$, hence the second term in (3.59) converges to

$$\left\| e^{(t-t_0)A\left(\frac{T}{n}\left[\frac{nt_0}{T}\right]\right)} U_n\left(\tfrac{T}{n}\left[\tfrac{nt_0}{T}\right], s\right) \right\| \xrightarrow{t \to t_0} 0.$$

An analogous consideration yields that also the third term in (3.59) becomes arbitrarily small. Thus we have shown assertion (c).

Our next step is to examine the behaviour of the sequence $\{W_n(t,s)\}_{n\in\mathbb{N}}$. We state the result in form of a lemma; its proof will be shown below.

Lemma 3.43. *Let $s, t \in [0,T]$, $s \leq t$. Then, with the definitions of Theorem 3.42 and under assumptions (i) to (iv),*

$$\operatorname*{s-lim}_{n\to\infty} W_n(t,s) = A(t)U(t,s)A(s)^{-1} =: W(t,s)$$

exists. Further, $W(t,s)$ is strongly continuous jointly in t and s and

$$\|W(t,s)\| \leq e^{N(t-s)},$$

where N is defined as in (3.49).

With this result we can show that $U(t,s)$ is indeed a time evolution for A, i.e. that it solves the Cauchy problem (b).
Let $y \in \mathcal{D}$. Then

$$A(t)U_n(t,s)y = W_n(t,s)A(s)y \xrightarrow{n\to\infty} W(t,s)A(s)y, \tag{3.60}$$

where the right hand side is uniformly strongly continuous in t and s, and besides

$$U_n(t,s)y \xrightarrow{n\to\infty} U(t,s)y. \tag{3.61}$$

Both strong limits (3.60) and (3.61) exist boundedly and uniformly in t and s. As $A(t)$ is closed as a consequence of the Hille-Yosida theorem, we conclude that

$$U(t,s)y \in \mathcal{D} \qquad \forall y \in \mathcal{D},$$

which proves assertion (d). Moreover, this implies

$$A(t)U(t,s)y = W(t,s)A(s)y. \tag{3.62}$$

Thus

$$\begin{aligned} U_n(t,s)y - y &= \int_s^t \tfrac{d}{dr} U_n(r,s)y\,dr \\ &= \int_s^t A\left(\tfrac{T}{n}\left[\tfrac{nr}{T}\right]\right) U_n(r,s)y\,dr \\ &= \int_s^t A\left(\tfrac{T}{n}\left[\tfrac{nr}{T}\right]\right) A(r)^{-1} W_n(r,s)A(s)y\,dr \\ &\xrightarrow{n\to\infty} \int_s^t W(r,s)A(s)y dr = \int_s^t A(r)U(r,s)y\,dr \end{aligned} \tag{3.63}$$

by (3.54), (3.62) and Lemma 3.43, which implies that

$$\tfrac{d}{dt}U(t,s)y = A(t)U(t,s)y. \tag{3.64}$$

This shows (b), and thus finally concludes the proof of Theorem 3.42. □

The proof of the auxiliary Lemma 3.43 is essentially taken from [35], Lemma 3.12. As in the proof of Theorem 3.42, we have slightly generalised the argument in order to comprise arbitrary $T \in \mathbb{R}_0^+$.

Proof of Lemma 3.43. We already know from (a) that $W_n^{(0)}(t,s)x = U_n(t,s)x$ converges for all $x \in X$ as $n \to \infty$. Our aim is now to show the convergence of $W_n^{(m)}(t,s)x$ for arbitrary m.
Let $m \in \mathbb{N}$ and $s,t \in [0,T]$, $s \le t$. With all objects defined as in Theorem 3.42, we introduce

$$\begin{aligned} f_n^{(m)}(t_1,\ldots,t_m) := \sum_{u_1=\frac{T}{n}\left[\frac{ns}{T}\right]+m}^{\frac{T}{n}\left[\frac{nt}{T}\right]} \cdots \sum_{u_m=\frac{T}{n}\left[\frac{ns}{T}\right]+1}^{u_{m-1}-1} & U_n\left(t,\tfrac{Tu_1}{n}\right)\tfrac{n}{T}C\left(\tfrac{Tu_1}{n},\tfrac{T(u_1-1)}{n}\right)U_n\left(\tfrac{Tu_1}{n},\tfrac{Tu_2}{n}\right)\cdot \\ & \cdot \cdots U_n\left(\tfrac{Tu_{m-1}}{n},\tfrac{Tu_m}{n}\right)\tfrac{n}{T}C\left(\tfrac{Tu_m}{n},\tfrac{T(u_m-1)}{n}\right)U_n\left(\tfrac{Tu_m}{n},s\right)x\,\cdot \\ & \cdot \mathbb{1}_{\left[\frac{T(u-1)}{n},\frac{Tu_1}{n}\right)}(t_1)\cdots \mathbb{1}_{\left[\frac{T(u_m-1)}{n},\frac{Tu_m}{n}\right)}(t_m), \end{aligned}$$

and for $s \le t_m \le \cdots \le t_1 \le t$,

$$f^{(m)}(t_1,\ldots,t_m) = U(t,t_1)C(t_1)U(t_1,t_2)C(t_2)\cdots U(t_{m-1},t_m)C(t_m)U(t_m,s)x, \tag{3.65}$$

with

$$C(t)x := \lim_{n\to\infty} nC(t,t-\tfrac{T}{n})x$$

as defined in assumption (iv). Further, we put

$$W^{(m)}(t,s)x := \int_s^t \int_s^{t_1} \cdots \int_s^{t_{m-1}} f^{(m)}(t_1,\ldots,t_m)dt_m\cdots dt_1. \tag{3.66}$$

The integral exists because $t \mapsto C(t)x$ is continuous according to assumption (iv). In the sequel, we will show that $W_n^{(m)}(t,s)x$ converges to $W^{(m)}(t,s)x$ as $n \to \infty$ for each m. To this end, we express $W_n^{(m)}(t,s)x$ as an integral. Consider first the case $m=1$. Then

$$\begin{aligned}
W_n^{(1)}(t,s)x &= \sum_{u=\left[\frac{ns}{T}\right]+1}^{\left[\frac{nt}{T}\right]} U_n\left(t,\tfrac{Tu}{n}\right) C\left(\tfrac{Tu}{n},\tfrac{T(u-1)}{n}\right) U_n\left(\tfrac{Tu}{n},s\right) x \\
&= \int\limits_{\left[\frac{ns}{T}\right]}^{\left[\frac{nt}{T}\right]} dt_1 \sum_{u=\left[\frac{ns}{T}\right]+1}^{\left[\frac{nt}{T}\right]} U_n\left(t,\tfrac{Tu}{n}\right) C\left(\tfrac{Tu}{n},\tfrac{T(u-1)}{n}\right) U_n\left(\tfrac{Tu}{n},s\right) \mathbb{1}_{[u-1,u)}(t_1)x \\
&= \int\limits_{\frac{T}{n}\left[\frac{ns}{T}\right]}^{\frac{T}{n}\left[\frac{nt}{T}\right]} dt_1\, f_n^{(1)}(t_1)
\end{aligned}$$

by substituting $t_1 \mapsto \frac{T}{n}t_1$. For generic $m \in \mathbb{N}$, we obtain

$$W_n^{(m)}(t,s) = \int\limits_{\frac{T}{n}\left(\left[\frac{ns}{T}\right]+m-1\right)}^{\frac{T}{n}\left[\frac{nt}{T}\right]} dt_1 \int\limits_{\frac{T}{n}\left(\left[\frac{ns}{T}\right]+m-2\right)}^{\frac{T}{n}\left[\frac{nt_1}{T}\right]} dt_2 \cdots \int\limits_{\frac{T}{n}\left[\frac{ns}{T}\right]}^{\frac{T}{n}\left[\frac{nt_{m-1}}{T}\right]} dt_m\, f_n^{(m)}(t_1,t_2,\ldots,t_m). \quad (3.67)$$

The $f_n^{(m)}(t_1,\ldots,t_m)$ are uniformly bounded: With (3.49), (3.50) and the consideration

$$\left\| \mathbb{1}_{\left[\frac{T(u-1)}{n},\frac{Tu}{n}\right)}(t_1)x \right\| \leq \left\| \int\limits_0^T dt_1 \mathbb{1}_{\left[\frac{T(u-1)}{n},\frac{Tu}{n}\right)}(t_1)x \right\| = \tfrac{T}{n}\left\|x\right\|,$$

we estimate

$$\begin{aligned}
&\left\| f_n^{(m)}(t_1,\ldots,t_m) \right\| \\
&\leq \sum_{u=\frac{T}{n}\left[\frac{ns}{T}\right]+m}^{\frac{T}{n}\left[\frac{nt}{T}\right]} \cdots \sum_{u=\frac{T}{n}\left[\frac{ns}{T}\right]+1}^{u_{m-1}-1} \left(\tfrac{n}{T}\right)^m \left\| C\left(\tfrac{Tu_1}{n},\tfrac{T(u_1-1)}{n}\right)\right\| \cdots \left\| C\left(\tfrac{Tu_m}{n},\tfrac{T(u_m-1)}{n}\right)\right\| \cdot \\
&\qquad \cdot \left\| \mathbb{1}_{\left[\frac{T(u_1-1)}{n},\frac{Tu_1}{n}\right)}(t_1)\right\| \cdots \left\| \mathbb{1}_{\left[\frac{T(u_m-1)}{n},\frac{Tu_m}{n}\right)}(t_m)\right\| \left\|x\right\| \\
&\leq \sum_{u=\frac{T}{n}\left[\frac{ns}{T}\right]+m}^{\frac{T}{n}\left[\frac{nt}{T}\right]} \cdots \sum_{u=\frac{T}{n}\left[\frac{ns}{T}\right]+1}^{u_{m-1}-1} \left(\tfrac{n}{T}\right)^m \left(\tfrac{NT}{n}\right)^m \left(\tfrac{T}{n}\right)^m \left\|x\right\|.
\end{aligned}$$

Each of the sums may contain at most n terms, as the whole interval $[0,T]$ is divided into n parts and $[s,t]$ is a subinterval of $[0,T]$. Hence we conclude

$$\left\| f_n^{(m)}(t_1,\ldots,t_m) \right\| \leq (NT)^m \left\|x\right\|. \quad (3.68)$$

Our next step is to show that $f_n^{(m)}(t_1,\dots,t_m) \to f^{(m)}(t_1,\dots,t_m)$ as $n\to\infty$. This is easiest to see for $m=1$:
For $t_1 \in [s,t]$, there is for every n some $l_n \in \{0,\dots,m_n(t,s)\}$ with $m_n(t,s)$ defined as in (3.48) such that

$$t_1 \in \Big[\tfrac{T}{n}\left(\left[\tfrac{ns}{T}\right]+l_n\right), \tfrac{T}{n}\left(\left[\tfrac{ns}{T}\right]+l_n+1\right)\Big).$$

Hence

$$\begin{aligned}
&\left\|f^{(1)}(t_1) - f_n^{(1)}(t_1)\right\| \\
&\quad= \Big\|U(t,t_1)C(t_1)U(t_1,s)x - U_n\Big(t, \tfrac{T}{n}\left(\left[\tfrac{ns}{T}\right]+l_n+1\right)\Big)\tfrac{n}{T}\,\cdot \\
&\qquad\qquad\cdot\, C\Big(\tfrac{T}{n}\left(\left[\tfrac{ns}{T}\right]+l_n+1\right), \tfrac{T}{n}\left(\left[\tfrac{ns}{T}\right]+l_n\right)\Big)U_n\Big(\tfrac{T}{n}\left(\left[\tfrac{ns}{T}\right]+l_n\right), s\Big)x\Big\|,
\end{aligned}$$

since all other contributions to the sum vanish. As $n\to\infty$, we have $\frac{T}{n}\left(\left[\frac{ns}{T}\right]+l_n+1\right)\to t_1$ because the width of the intervals of the partition becomes arbitrarily small in this limit. The convergence follows from this as $(t,s)\mapsto U(t,s)x$ and $t\mapsto C(t)x$ are continuous,

$$\sup_{\substack{s,t\in[0,T]\\ s\le t}} \|U(t,s)x - U_n(t,s)x\| \xrightarrow{n\to\infty} 0$$

and

$$\sup_{t\in\left[\frac{T}{n},T\right]} \left\|\tfrac{n}{T}C\left(t,t-\tfrac{T}{n}\right)x - C(t)x\right\| \xrightarrow{n\to\infty} 0$$

for all $x\in X$. The case $m\neq 1$ works analogously.

This result and the uniform boundedness (3.68) of $f_n^{(m)}(t_1,\dots,t_m)$ enable us to apply the theorem of dominated convergence. With (3.67) we obtain

$$\begin{aligned}
W_n^{(m)}(t,s)x &= \int\limits_{\frac{T}{n}\left(\left[\frac{ns}{T}\right]+m-1\right)}^{\frac{T}{n}\left[\frac{nt}{T}\right]} dt_1 \cdots \int\limits_{\frac{T}{n}\left[\frac{ns}{T}\right]}^{\frac{T}{n}\left[\frac{nt_{m-1}}{T}\right]} dt_m\, f_n^{(m)}(t_1,\dots,t_m) \\
&\xrightarrow{n\to\infty} \int\limits_s^t dt_1 \cdots \int\limits_s^{t_{m-1}} dt_m\, f^{(m)}(t_1,\dots,t_m) = W^{(m)}(t,s)x,
\end{aligned} \tag{3.69}$$

where we have exploited that $\frac{T}{n}\left[\frac{nt}{T}\right] \xrightarrow{n\to\infty} t$ and $\frac{T}{n}\left(\left[\frac{ns}{T}\right]+p\right) \xrightarrow{n\to\infty} s$ for $p\in\mathbb{N}$.

Taking $n\to\infty$ implies that $m_n(t,s)\to\infty$ in (3.47) due to (3.48). Therefore,

$$\begin{aligned}
W(t,s)x &= \lim_{n\to\infty} W_n(t,s)x \\
&= \lim_{n\to\infty} \Big(\mathbb{1} + C\left(t, \tfrac{T}{n}\left[\tfrac{nt}{T}\right]\right)\Big) \sum_{m=0}^{\infty} W_n^{(m)}(t,s)\Big(\mathbb{1} + C\left(\tfrac{T}{n}\left[\tfrac{ns}{T}\right]\right), s\Big)x \\
&= \sum_{m=0}^{\infty} W^{(m)}(t,s)
\end{aligned} \tag{3.70}$$

exists according to (3.69) and (3.52), and

$$\|W(t,s)x\| = \lim_{n\to\infty} \|W_n(t,s)x\| \le e^{N(t-s}\,\|x\|\,.$$

Moreover, $W(t,s)$ is uniformly continuous jointly in t and s because $(s,t) \mapsto W^{(m)}(t,s)x$ is continuous and the series in (3.70) converges uniformly. □

When applying YOSIDA's theorem to physical problems, assumption (iv) is usually the most cumbersome to verify. There is however a recent work by GRIESEMER and SCHMID, which shows that this rather involved formulation is equivalent to a much simpler condition.

Lemma 3.44. *Assumption (iv) in Theorem 3.42 is equivalent to*

(iv′) $t \mapsto A(t)x$ is continuously differentiable with respect to the norm of X for every $x \in \mathcal{D}$.

Proof. [36], Theorem 2.2. □

It finally remains to establish the unitarity of the time evolution operator, whose existence and uniqueness under suitable assumptions has been proved in Theorems 3.38, 3.41 and 3.42. To this end we quote (the main part of) Proposition 3.16. from [35] and also present the proof as it is given there, adapted to the general case where T is not bound to equal 1. With the sign convention of (3.40) as used in YOSIDA's theorem we find

Theorem 3.45. *Let $A(t) : X \supseteq \mathcal{D} \to X$ be a linear map for each $t \in [0,T]$, generating the evolution operator $\{U(t,s)\}_{0\le s\le t\le T}$.*

(a) Let $t \mapsto A(t)x$ be norm-continuous for each $x \in \mathcal{D}$. Then $U(t,s)$ is isometric for all $s,t \in [0,T]$, $s \le t$, if $A(t)$ is skew symmetric for each $t \in [0,T]$.

(b) Let $t \mapsto A(t)x$ be continuously differentiable for each $x \in \mathcal{D}$. Then $U(t,s)$ is unitary for all $s,t \in [0,T]$, $s \le t$, if $A(t)$ is skew self-adjoint for each $t \in [0,T]$.

Proof. For part (a), let $x,y \in \mathcal{D}$. Then due to the skew symmetry of $A(t)$,

$$\tfrac{d}{dt}\langle U(t,s)x, U(t,s)y\rangle = \langle A(t)U(t,s)x, U(t,s)y\rangle - \langle A(t)U(t,s)x, U(t,s)y\rangle = 0,$$

and hence

$$\langle U(t,s)x, U(t,s)y\rangle = \langle U(t,s)x, U(t,s)y\rangle\,\big|_{t=s} = \langle x,y\rangle$$

for all $x,y \in \mathcal{D}$ and $s,t \in [0,T]$, $s \le t$. This shows the isometry of the time evolution.

To prove part (b), it remains to show that

$$U(t,s)U(t,s)^* = \mathbb{1}. \tag{3.71}$$

Our strategy will be the following: we approximate $U(t,s)$ by $U_n(t,s)$ as in Theorems 3.38 and 3.42. Noting that $U_n(t,s)$ is unitary for each $n \in \mathbb{N}$, we conclude that also the limit $U(t,s)$ must be a unitary operator. This conclusion can however not be drawn immediately, as the strong limit of a sequence of unitary operators is always isometric but not necessarily unitary[7]. Therefore we prove first that

$$U(t,s)U_n(t,s)^*x \xrightarrow{n\to\infty} x. \tag{3.72}$$

This will be achieved by observing that

$$U(t,s)U_n(t,s)^*x - x = U_n(t,r)U(r,s)U_n(t,s)^*x\Big|_{r=s}^{r=t}, \tag{3.73}$$

which can be estimated employing the methods of the proof of Theorem 3.42. From (3.72) we deduce then that (3.71) holds true.
To make these ideas rigorous, we define

$$\begin{aligned}
\widetilde{A}(t) &:= A(t) - \mathbb{1},\\
\widetilde{U}_n(t,s) &:= U_n(t,s)e^{-(t-s)},\\
\widetilde{U}(t,s) &:= U(t,s)e^{-(t-s)},\\
\widetilde{W}(t,s) &:= \widetilde{A}(t)\widetilde{U}(t,s)\widetilde{A}(s)^{-1},\\
\widetilde{V}_n(t,s) &:= \widetilde{A}(s)U_n(t,s)^*\widetilde{A}(t)^{-1}\\
\widetilde{C}(t,s) &:= \widetilde{A}(t)\widetilde{A}(s)^{-1} - \mathbb{1}.
\end{aligned}$$

$U_n(t,s)$ is clearly unitary because each of the factors in (3.41) is unitary as a consequence of Stone's theorem. From the proof of Theorem 3.42 we infer that

$$\widetilde{U}_n(t,s)e^{(t-s)}x = U_n(t,s)x \xrightarrow{n\to\infty} U(t,s)x = \widetilde{U}_n(t,s)e^{(t-s)}x \tag{3.74}$$

for all $x \in X$, and accordingly

$$\begin{aligned}
\langle U(t,s)U_n(t,s)^*x, y\rangle &= \langle x, U_n(t,s)U(t,s)^*y\rangle\\
&\xrightarrow{n\to\infty} \langle x, U(t,s)U(t,s)^*y\rangle = \langle U(t,s)U(t,s)^*x, y\rangle
\end{aligned} \tag{3.75}$$

for all $x, y \in X$. Using the skew self-adjointness of $A(t)$, we expand $\widetilde{V}_n(t,s)$ analogously to (3.44) and (3.45) and obtain

$$\begin{aligned}
\widetilde{V}_n(t,s) &= \widetilde{A}(s)e^{\left(s-\frac{T}{n}\left(\left[\frac{ns}{T}\right]+1\right)\right)A\left(\frac{T}{n}\left[\frac{ns}{T}\right]\right)}e^{-\frac{T}{n}A\left(\frac{T}{n}\left(\left[\frac{ns}{T}\right]+1\right)\right)}\cdots e^{\left(\frac{T}{n}\left[\frac{nt}{T}\right]-t\right)A\left(\frac{T}{n}\left[\frac{nt}{T}\right]\right)}\widetilde{A}(t)^{-1}\\
&= \Big(\mathbb{1}+\widetilde{C}\left(s,\tfrac{T}{n}\left[\tfrac{ns}{T}\right]\right)\Big)e^{\left(s-\frac{T}{n}\left(\left[\frac{ns}{T}\right]+1\right)\right)A\left(\frac{T}{n}\left[\frac{ns}{T}\right]\right)}\Big(\mathbb{1}+\widetilde{C}\left(\tfrac{T}{n}\left[\tfrac{ns}{T}\right],\tfrac{T}{n}\left(\left[\tfrac{ns}{T}\right]+1\right)\right)\Big)\cdot\\
&\quad\cdot e^{-\frac{T}{n}A\left(\frac{T}{n}\left(\left[\frac{ns}{T}\right]+1\right)\right)}\cdots e^{\left(\frac{T}{n}\left[\frac{nt}{T}\right]-t\right)A\left(\frac{T}{n}\left[\frac{nt}{T}\right]\right)}\Big(\mathbb{1}+\widetilde{C}\left(\tfrac{T}{n}\left[\tfrac{nt}{T}\right],t\right)\Big).
\end{aligned}$$

We note that the above product contains $m_n(t,s)+2$ terms of the form $\big(\mathbb{1}+\widetilde{C}(\cdot,\cdot)\big)$, with $m_n(t,s)$ as in (3.48). Analogously to (3.49), we define

$$\widetilde{N} := \sup_{\substack{s,t\in[0,T]\\ s\neq t}} \left\|\tfrac{1}{t-s}\widetilde{C}(t,s)\right\| \tag{3.76}$$

[7] See [45, Ch. II], Remark 4.10.

and, using the fact that $A(t)$ generates a unitary group for each t, estimate

$$\left\|\widetilde{V}_n(t,s)\right\| \leq \left(1+\tfrac{\widetilde{N}T}{n}\right)^{m_n(t,s)+2}. \tag{3.77}$$

By definition (3.48), $m_n(t,s)$ is the largest integer such that $m_n(t,s) \leq \left[\frac{nt}{T}\right] - \left[\frac{ns}{T}\right]$. As $\left[\frac{nt}{T}\right] - \left[\frac{ns}{T}\right] \leq \frac{n}{T}(t-s)+1$,

$$m_n(t,s) \leq \tfrac{n}{T}(t-s)+1,$$

and we conclude

$$\begin{aligned}\left\|\widetilde{V}_n(t,s)\right\| &\leq \left(1+\tfrac{\widetilde{N}T}{n}\right)^{n+3} \\ &\leq (1+\tfrac{\widetilde{N}T}{n})^3 e^{\widetilde{N}(t-s)}.\end{aligned} \tag{3.78}$$

We can now proceed to proving (3.72). For $r \in (s,t)$ and $r \neq \frac{j}{n}T$, $j = 1,\ldots,n$, (r lying between s and t but not coinciding with any of the borders of the enclosed subintervals),

$$\begin{aligned}&\tfrac{d}{dr}\Big(U_n(t,r)U(r,s)U_n(t,s)^*x\Big)\\ &\qquad= U_n(t,r)\left(A(r) - A\left(\tfrac{T}{n}\left[\tfrac{nr}{T}\right]\right)\right)U(r,s)U_n(t,s)^*x\\ &\qquad= U_n(t,r)\Big(\mathbb{1} - \widetilde{A}\left(\tfrac{T}{n}\left[\tfrac{nr}{T}\right]\right)\widetilde{A}(r)^{-1}\Big)\widetilde{A}(r))U(r,s)U_n(t,s)^*x\\ &\qquad= -\widetilde{C}\left(\tfrac{T}{n}\left[\tfrac{nr}{T}\right],r\right)\widetilde{A}(r)\widetilde{U}(r,s)\widetilde{A}(s)^{-1}e^{r-s}\widetilde{A}(s)U_n(t,s)^*\widetilde{A}(t)^{-1}\widetilde{A}(t)x\\ &\qquad= -\widetilde{C}\left(\tfrac{T}{n}\left[\tfrac{nr}{T}\right],r\right)\widetilde{W}(r,s)e^{r-s}\widetilde{V}_n(t,s)\widetilde{A}(t)x.\end{aligned}$$

The norm of $\widetilde{W}(t,s)$ can be estimated analogously to the reasoning in (3.44) until (3.52) and Lemma 3.43, yielding

$$\left\|\widetilde{W}(t,s)\right\| \leq \left(1+\widetilde{N}\right)^2 e^{\widetilde{N}(t-s)}. \tag{3.79}$$

Hence we gather from (3.76), (3.78) and (3.79) that the map $r \mapsto U_n(t,r)U(r,s)U_n(t,s)^*x$ is continuously differentiable for r as specified above. In particular,

$$\begin{aligned}\left\|\tfrac{d}{dr}\Big(U_n(t,r)U(r,s)U_n(t,s)^*x\Big)\right\| &\leq \tfrac{\widetilde{N}T}{n}(1+\widetilde{N})^2\left(1+\tfrac{\widetilde{N}T}{n}\right)^3 e^{(\widetilde{N}+1)(r-s)}e^{\widetilde{N}(t-s)}\left\|\widetilde{A}(t)x\right\|\\ &\leq \tfrac{\widetilde{N}T}{n}(1+\widetilde{N})^2\left(1+\tfrac{\widetilde{N}T}{n}\right)^3 e^{(2\widetilde{N}+1)T}\left\|\widetilde{A}(t)x\right\|.\end{aligned}$$

As this is clearly bounded uniformly in n we conclude, recalling (3.73), that

$$\begin{aligned}\|U(t,s)U_n(t,s)^*x - x\| &= \left\|\int_s^t \tfrac{d}{dr}\Big(U_n(t,r)U(r,s)U_n(t,s)^*x\Big)dr\right\|\\ &\leq \tfrac{\widetilde{N}T}{n}(1+\widetilde{N})^2\left(1+\tfrac{\widetilde{N}T}{n}\right)^3 e^{(2\widetilde{N}+1)T}\left\|\widetilde{A}(t)x\right\|(t-s)\\ &\longrightarrow 0 \qquad \text{as } n\to\infty,\end{aligned}$$

hence

$$U(t,s)U_n(t,s)^*x \xrightarrow{n\to\infty} x.$$

Thus it holds for all $x \in \mathcal{D}$, $y \in X$, $s,t \in [0,T]$, $s \leq t$, that

$$\langle U(t,s)U(t,s)^*x, y\rangle = \lim_{n\to\infty}\langle U(t,s)U_n(t,s)^*x, y\rangle = \langle x, y\rangle, \tag{3.80}$$

which finally implies (3.71). $\square$

3.5 Inequalities

In the last section of this preparatory chapter we introduce two forms of Gronwall's lemma. It provides us with a tool to bound a function satisfying a certain differential (3.46) or integral (3.47) inequality by the solution of the corresponding differential or integral equation.

Lemma 3.46. (Gronwall) *Let $T > 0$, $f : [0, T] \to \mathbb{R}$ continuous and*

$$\frac{d}{dt} f(t) \leq g(t) f(t) + h(t)$$

for integrable functions $g, h : [0, T] \to \mathbb{R}_0^+$. Then

$$f(t) \leq \left[f(0) + \int_0^t h(s) ds \right] e^{\int_0^t g(s) ds}$$

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

Proof. [37], Appendix B.2j. □

Lemma 3.47. (Gronwall-Bellman) *Let u and f be continuous and non-negative functions defined on $J = [\alpha, \beta]$, $\alpha, \beta \in \mathbb{R}$. Let c be a non-negative constant and*

$$u(t) \leq c + \int_\alpha^t f(s) u(s) ds \ \ , \ t \in J. \tag{3.81}$$

Then

$$u(t) \leq c \exp \left\{ \int_\alpha^t f(s) ds \right\} \ \ , \ t \in J. \tag{3.82}$$

Proof. [38], Theorem 1.2.2. □

4 Existence and Convergence of the Time Evolutions

In Chapter 2, we have motivated the semiclassical Hamiltonian $H_\lambda(t)$ (2.3) and argued that it can be approximated by $H_\infty(t)$ (2.7) if the wavelength of the external field is sufficiently large with respect to the atomic length scale. With the conventions $e = \hbar = 1$ and $m = \frac{1}{2}$, (2.3) and (2.7) read

$$
\begin{aligned}
H_\lambda(t) &= \left(-i\nabla - \tfrac{1}{c}\mathbf{A}_\lambda(\cdot, t)\right)^2 + V(\cdot), &(4.1)\\
H_\infty(t) &= \left(-i\nabla - \tfrac{1}{c}\mathbf{A}_\lambda(0, t)\right)^2 + V(\cdot). &(4.2)
\end{aligned}
$$

Here, $V : \mathbb{R}^d \to \mathbb{R}$ is a real-valued function and $V(\cdot)$ denotes the respective multiplication operator on $L^2(\mathbb{R}^d)$. For convenience, we will in the following refrain from the distinction between function and multiplication operator and use the notation $V \equiv V(\cdot)$.

Now we make the heuristic argument from Chapter 2 rigorous. First, we phrase the above demand for well separated length scales in a more precise way in form of a limit. We are free to choose between two options: either we consider λ to be fixed and let the separation between electron and nucleus tend towards zero; or we proceed conversely, keeping the coordinates of the electron undisturbed and sending the wavelength towards infinity. We will in the sequel take the second path and examine the simultaneous limit $\lambda, c \to \infty$ such that the frequency ω of the radiation, and consequently the energy transferred to the atom, remains constant.

The next step is to clarify which criterion distinguishes a good approximation. Assume we start at time t_0 with some initial wave function ψ and let it evolve separately under the time evolutions $U_\lambda(t, t_0)$ and $U_\infty(t, t_0)$, generated respectively by $H_\lambda(t)$ and $H_\infty(t)$. It seems sensible to speak of a good approximation if these evolutions do not differ considerably: the *distance* between $U_\lambda(t, t_0)\psi$ and $U_\infty(t, t_0)\psi$ should be small in order for the dipole approximation to be valid. As the $L^2(\mathbb{R}^d)$-norm provides a natural choice of distance, we infer that the quality of the approximation should be determined by

$$\|(U_\lambda(t, t_0) - U_\infty(t, t_0))\psi\| .$$

Hence our goal will be to prove that the exact time evolution $U_\lambda(t, t_0)$ converges strongly to the approximated time evolution $U_\infty(t, t_0)$ in the limit $\lambda, c \to \infty$ with ω kept constant.

In Chapter 2, we have already invoked the example of a plane electromagnetic wave (2.5). Noting that the dependence on λ is merely in the fraction $\frac{\mathbf{x}}{\lambda}$ and that ω occurs coupled to t, we write the external field $\mathbf{A}_\lambda(\mathbf{x}, t)$ such that it has no hidden dependencies on λ, c or ω,

$$\mathbf{A}_\lambda(\mathbf{x}, t) = \tfrac{c}{\omega}\mathbf{a}\left(\tfrac{\mathbf{x}}{\lambda}, \omega t\right), \tag{4.3}$$

with $\mathbf{a}$ independent of said variables. In Section 4.1.2, we will see that at least in the two experimentally most relevant cases – plane waves and laser pulses – this form can be achieved. The representation (4.3) is advantageous as it allows us to perform the limit $\lambda, c \to \infty$ in a more straightforward way. Moreover, insertion of (4.3) into the Hamiltonians (4.1) and (4.2) results in

$$H_\lambda(\mathbf{x}, t) = \left(-i\nabla - \tfrac{1}{\omega}\mathbf{a}\left(\tfrac{\mathbf{x}}{\lambda}, \omega t\right)\right)^2 + V(\mathbf{x}), \tag{4.4}$$

$$H_\infty(\mathbf{x}, t) = \left(-i\nabla - \tfrac{1}{\omega}\mathbf{a}\left(0, \omega t\right)\right)^2 + V(\mathbf{x}). \tag{4.5}$$

Hence $H_\lambda(t)$ does not depend on c any more, and the dependence on λ is restricted to the first argument of $\mathbf{a}$.

Thus prepared, we proceed to the main theorem of this chapter, which establishes in particular the convergence of the time evolutions in the limit of infinite wavelengths.

Theorem 4.1. *Let $T > 0$ and define $H_\lambda(t)$ and $H_\infty(t)$ as in (4.1) and (4.2). Assume that*

(A1) $V \in L^2_{\text{loc}}(\mathbb{R}^d)$ *and* $V << -\Delta$,

(A2) $\mathbf{A}_\lambda(\mathbf{x}, t)$ *can be written as in (4.3), with* $\mathbf{a} \in \mathcal{C}^2(\mathbb{R}^{d+1}, \mathbb{R}^d)$ *independent of* λ, ω, c,

(A3) $\nabla \cdot \mathbf{a}(\mathbf{x}, t) = 0$,

(A4) $\left\|\partial_t^j a_i(\cdot, t)\right\|_\infty \leq C < \infty$ *uniformly in* t *for* $i = 1, \ldots, d$ *and* $j = 0, 1, 2$.

Then for $t \in [0, T]$,

(1a) $H_\lambda(t)$ *and* $H_\infty(t)$ *are self-adjoint on* $\mathcal{D} \equiv \mathcal{D}(H_\lambda(t)) = \mathcal{D}(H_\infty(t)) = H^2(\mathbb{R}^d)$,

(1b) $H_\lambda(t)$ *and* $H_\infty(t)$ *each generate a unique family of unitary evolution operators* $\{U_\lambda(t, t_0)\}_{0 \leq t_0 \leq t}$ *and* $\{U_\infty(t, t_0)\}_{0 \leq t_0 \leq t}$*, respectively,*

(1c) $U_\lambda(t, t_0)$ *and* $U_\infty(t, t_0)$ *are strongly continuous jointly in* t *and* t_0,

(1d) $U_\lambda(t, t_0)$ *and* $U_\infty(t, t_0)$ *leave* $\mathcal{D}$ *invariant.*

Furthermore,

(2) for $\psi \in L^2(\mathbb{R}^d)$, $0 \leq t_0 \leq t < T$,

$$\lim_{\substack{\lambda \to \infty \\ c \to \infty \\ \omega = const.}} \left\|\left(U_\lambda(t, t_0) - U_\infty(t, t_0)\right)\psi\right\| = 0,$$

where the limits $\lambda \to \infty$, $c \to \infty$ *are taken such that* ω *remains constant.*

4.1 On the Assumptions

To assure the physical relevance of Theorem 4.1, we first examine the assumptions. We show that the possible potentials conclude N-electron atoms, even molecules, and verify that the electric fields permitted by (A2)-(A4) describe the experimentally relevant cases.

4.1.1 Potential

A molecule with N electrons and M nuclei in three dimensions is described by the potential

$$
\begin{aligned}
V_{\mathrm{mol}}(\mathbf{x}_1, ..., \mathbf{x}_N; \mathbf{R}_1, ..., \mathbf{R}_M) = &\sum_{1 \leq i < j \leq N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} - \sum_{i=1}^{N} \sum_{j=1}^{M} \frac{Z_j}{|\mathbf{x}_i - \mathbf{R}_j|} \\
&+ \sum_{1 \leq i < j \leq M} \frac{Z_i Z_j}{|\mathbf{R}_i - \mathbf{R}_j|} ,
\end{aligned} \tag{4.6}
$$

where $\mathbf{x}_i$ are the positions of the electrons, $\mathbf{R}_i$ the positions of the nuclei and Z_i the atomic numbers of the respective atoms. For $M = 1$, (4.6) describes a single atom with N electrons. The proof that V_{mol} fulfils assumption (A1) arises from the following two theorems from the textbook of Reed and Simon [14].

Theorem 4.2. *Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ be real-valued. Then $V << -\Delta$, where $-\Delta$ denotes the three-dimensional Laplace operator.*

Proof. [14], Theorem X.15. □

Here, $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ means that there exist $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$ such that $V = V_1 + V_2$. Clearly, $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \subseteq L^2_{\mathrm{loc}}(\mathbb{R}^3)$ – the L^∞-part is square integrable on every compactum, and the L^2-part is naturally everywhere square integrable. In other words, $L^2_{\mathrm{loc}}(\mathbb{R}^3)$ permits an L^2-singularity on every compact set whereas for elements of $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, the singularity is restricted to one closed ball. The most relevant example is the Coulomb potential, which we will analyse in detail shortly.

Theorem 4.3. *Let $\{V_k\}_{1 \leq k \leq N}$ be a collection of real-valued measurable functions with $V_k \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for each k. Let $V_k(\mathbf{x}_k)$ be the multiplication operator on $L^2(\mathbb{R}^{3N})$ obtained by choosing $\mathbf{x}_k$ to be three coordinates of $\mathbb{R}^{3N}$. Then $\sum_{k=1}^N V_k(\mathbf{x}_k) << -\Delta$, where $-\Delta$ denotes the Laplace operator on $\mathbb{R}^{3N}$.*

Proof. [14], Theorem X.16. □

Let us consider the hydrogen atom with its nucleus at $\mathbf{R} = 0$. Assumption (A1) is fulfilled because

$$V_{\mathrm{hydrogen}}(\mathbf{x}) = -\frac{1}{|\mathbf{x}|} = -\mathbb{1}_{\{|\mathbf{x}| \leq 1\}} \frac{1}{|\mathbf{x}|} - \mathbb{1}_{\{|\mathbf{x}| > 1\}} \frac{1}{|\mathbf{x}|},$$

where

$$\left\| -\mathbb{1}_{\{|\mathbf{x}| \leq 1\}} \frac{1}{|\mathbf{x}|} \right\|_2 = 4\pi$$

and

$$\left\| -\mathbb{1}_{\{|\mathbf{x}| > 1\}} \frac{1}{|\mathbf{x}|} \right\|_\infty = 1,$$

hence the first summand is in $L^2(\mathbb{R}^3)$ and the second one in $L^\infty(\mathbb{R}^3)$. V_{hydrogen} is thus an element of $L^2_{\mathrm{loc}}(\mathbb{R}^3)$ and, as a consequence of Theorem 4.2, $V_{\mathrm{hydrogen}} << -\Delta$.

The infinitesimal boundedness of an atom or molecule described by (4.6) is given by Theorem 4.3: Define

$$V_{1,ij}(\mathbf{x}_i - \mathbf{x}_j) \equiv \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}\,, \tag{4.7}$$

$$V_{2,ij}(\mathbf{x}_i - \mathbf{R}_j) \equiv \frac{Z_j}{|\mathbf{x}_i - \mathbf{R}_j|}\,, \tag{4.8}$$

$$V_{3,ij}(\mathbf{R}_i - \mathbf{R}_j) \equiv \frac{Z_i Z_j}{|\mathbf{R}_i - \mathbf{R}_j|}\,. \tag{4.9}$$

Then

$$V_{\mathrm{mol}} = \sum_{1\le i<j\le N} V_{1,ij} + \sum_{i=1}^{N}\sum_{j=1}^{M} V_{2,ij} + \sum_{1\le i<j\le M} V_{3,ij},$$

and analogously to the potential of the hydrogen atom,

$$V_{1,ij}, V_{2,ij}, V_{3,ij} \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$$

for $1 \le i \le N$, $1 \le j \le M$.

One might be inclined to draw the conclusion that the dipole approximation may be applied to electrons in external fields which are confined to any atomic or molecular potential. This is however only partly true: if the electron in question interacts with other electrons, and besides with nuclei that may not be considered static, the Hamiltonian $H_\lambda(t)$ does not describe the situation sufficiently well any more. In addition to the external electromagnetic field, we would then have to take into consideration the fields generated by the other particles, which influence the electron's motion as well. Hence, in practice, the dipole approximation will only be applied if this influence is negligible, for instance in Rydberg atoms or atoms with a single valence electron.

4.1.2 External Field

Let us now examine the assumption on the external electromagnetic field. We work in the Coulomb gauge, hence assumption (A3) is always fulfilled. Whereas assumption (A2) is needed for the scaling, it is physically reasonable to assume (A4): it states that the vector potential, the electric field an the latter's time derivative – related to the rotation of the magnetic field – are uniformly bounded during the compact time interval $[0, T]$.

As a first example we consider plane wave solutions of the vacuum Maxwell equations,

$$\mathbf{E}(\mathbf{x}, t) = E\cos(\mathbf{k}\cdot\mathbf{x} - \omega t)\hat{\varepsilon}, \quad \mathbf{k}\cdot\hat{\varepsilon} = 0, \tag{4.10}$$

where $\omega = \frac{2\pi c}{\lambda}$ and $|\mathbf{k}| = \frac{2\pi}{\lambda}$. In practice, such electric fields are realised by *continuous wave lasers*. The electric field (4.10) is generated through (2.2) by the vector potential

$$\mathbf{A}_\lambda(\mathbf{x}, t) = \frac{cE}{\omega}\sin\left(\frac{2\pi}{\lambda}\hat{k}\cdot\mathbf{x} - \omega t\right)\hat{\varepsilon}$$

as can easily be verified. Putting

$$\mathbf{a}(\mathbf{x}, t) = E\sin(2\pi\hat{k}\cdot\mathbf{x} - t)\hat{\varepsilon},$$

we see that assumption (A2) is obviously true. Assumption (A3) is easily verified because

$$\nabla \cdot \mathbf{a}(\mathbf{x}, t) = 2\pi \cos(2\pi \hat{k} \cdot \mathbf{x} - t) \hat{k} \cdot \hat{\varepsilon} = 0$$

due to (4.10). Assumption (A4) is also clear as

$$\left\| \partial_t^j a^i(\cdot, t) \right\|_\infty \leq |E| < \infty.$$

Hence plane electromagnetic waves are covered by Theorem 4.1.

Another relevant solution of the sourceless Maxwell equation are *laser pulses*,

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{E}_0(\mathbf{x}, t) \cos(\mathbf{k} \cdot \mathbf{x} - \omega t),$$

with vector potential

$$\mathbf{A}_\lambda(\mathbf{x}, t) = -c \int_{-\infty}^{t} \mathbf{E}_0(\mathbf{x}, s) \cos(\mathbf{k} \cdot \mathbf{x} - \omega s) ds.$$

For practical purposes, we consider Laser pulses with Gaussian envelope,

$$\mathbf{E}(\mathbf{x}, t) = E e^{-(\mathbf{k} \cdot \mathbf{x} - \omega t)^2} \cos\left(\mathbf{k} \cdot \mathbf{x} - \omega t\right) \hat{\varepsilon}, \quad \mathbf{k} \cdot \hat{\varepsilon} = 0,$$

with $\mathbf{k}$, ω as before. Substituting $s \mapsto \omega s$, we obtain

$$\mathbf{A}_\lambda(\mathbf{x}, t) = \tfrac{c}{\omega} \mathbf{a}\left(\tfrac{\mathbf{x}}{\lambda}, \omega t\right) = -\tfrac{c}{\omega} E \int_{-\infty}^{\omega t} e^{-\left(\frac{2\pi}{\lambda} \hat{k} \cdot \mathbf{x} - s\right)^2} \cos\left(\tfrac{2\pi}{\lambda} \hat{k} \cdot \mathbf{x} - s\right) \hat{\varepsilon}\, ds$$

and

$$\mathbf{a}(\mathbf{x}, t) = -E \int_{-\infty}^{t} e^{-(2\pi \hat{k} \cdot \mathbf{x} - s)^2} \cos(2\pi \hat{k} \cdot \mathbf{x} - s) \hat{\varepsilon}\, ds,$$

which shows the viability of assumption (A2). Assumption (A3) holds as well because

$$\begin{aligned} \nabla \cdot \mathbf{a}(\mathbf{x}, t) = 4\pi E &\int_{-\infty}^{t} (2\pi \hat{k} \cdot \mathbf{x} - s) e^{-(2\pi \hat{k} \cdot \mathbf{x} - s)^2} \cos(2\pi \hat{k} \cdot \mathbf{x} - s) \hat{k} \cdot \hat{\varepsilon}\, ds \\ + 2\pi E &\int_{-\infty}^{t} \sin(2\pi \hat{k} \cdot \mathbf{x} - s) e^{-(2\pi \hat{k} \cdot \mathbf{x} - s)^2} \hat{k} \cdot \hat{\varepsilon}\, ds = 0 \end{aligned}$$

due to (4.10). In order to verify assumption (A4), we substitute $u = 2\pi \hat{k} \cdot \mathbf{x} - s$, which yields

$$\mathbf{a}(\mathbf{x}, t) = -E \int_{2\pi \hat{k} \cdot \mathbf{x} - t}^{\infty} e^{-u^2} \cos(u) \hat{\varepsilon}\, du,$$

hence

$$\begin{aligned}
|a^i(\mathbf{x},t)| &\leq |E| \int\limits_{2\pi\hat{k}\cdot\mathbf{x}-t}^{\infty} e^{-u^2} du \leq |E| \int\limits_{-\infty}^{\infty} e^{-u^2} du = \sqrt{\pi}|E|, \\
|\partial_t a^i(\mathbf{x},t)| &\leq \left| E e^{-(2\pi\hat{k}\cdot\mathbf{x}-t)^2} \cos(2\pi\hat{k}\cdot\mathbf{x}-t) \right| \leq |E|, \\
|\partial_t^2 a^i(\mathbf{x},t)| &\leq |E| \left(2|2\pi\hat{k}\cdot\mathbf{x}-t|+1\right) e^{-|2\pi\hat{k}\cdot\mathbf{x}-t|^2} \leq 2e^{-\frac{1}{4}}|E|.
\end{aligned} \tag{4.11}$$

The last step in (4.11) follows by observing that

$$f(y) \equiv (2y+1)e^{-y^2}$$

has a global maximum at $y = \frac{1}{2}$, hence

$$f(y) \leq 2e^{-\frac{1}{4}}.$$

The remainder of this chapter is devoted to the proof of Theorem 4.1. There are basically two paths to take: Recalling Section 3.4, we know that there exist two approaches establishing the existence of the time evolution operators for unbounded time-dependent Hamiltonians: Theorems 3.38 and 3.41 by Kato, and Yosida's Theorem 3.42. The proof of our Theorem 4.1 can be achieved using either, and both ways of proving it are of comparable complexity. We will show Part 1 first using Kato's framework, as it is the original and more general one. In Section 4.3, we then present a proof based on Yosida's theorem. A crucial ingredient for both proofs is the uniform equivalence of the graph norm of the Hamiltonians and the Sobolev norm, which is shown in Section 4.2.2.
Part 2 relies on Part 1 as well as on an estimate of the kinetic energy. We prove first an exponential upper bound, which again can be achieved using either Kato's or Yosida's methods and also emerges directly from the Schrödinger equation (Section 4.4). For the time evolution generated by $H_\infty(t)$, this can be improved to a uniform bound. As a consequence, the proof of Part 2 reduces essentially to an application of the theorem of dominated convergence.

An earlier version of this proof can be found in [12, 13]. In this work, the authors use Theorem X.70 from Reed's and Simon's textbook, which essentially corresponds to Yosida's theorem. Although our proof is considerably different, we have adopted some features from said work, in particular the proof of Part (1a) and Lemma 4.5.

4.2 Proof of Part 1 using Kato's Theorems

We first prove assertion (1a) of Theorem 4.1 using the Kato-Rellich Theorem (Theorem 3.8). Assertions (1b) to (1d) follow from Kato's Theorems (Theorem 3.38 and Theorem 3.41).

4.2.1 Self-Adjointness of the Hamiltonians

We show now assertion (1a) of Theorem 4.1. This part of the proof is entirely taken from [12, 13], but we present the steps in considerably greater detail.

Define the multiplication operator

$$\begin{aligned} W_\lambda(t) : L^2(\mathbb{R}^d) \supseteq \mathcal{D}(W_\lambda(t)) &\longrightarrow L^2(\mathbb{R}^d) \\ \psi(\mathbf{x}) &\longmapsto W_\lambda(\mathbf{x},t)\psi(\mathbf{x}), \end{aligned}$$

where

$$\begin{aligned} W_\lambda(\mathbf{x},t) &= \tfrac{2i}{c}\mathbf{A}_\lambda(\mathbf{x},t)\cdot\nabla + \tfrac{1}{c^2}\mathbf{A}_\lambda(\mathbf{x},t)^2 + V(\mathbf{x}) \\ &= \tfrac{2i}{\omega}\mathbf{a}\left(\tfrac{\mathbf{x}}{\lambda},\omega t\right)\cdot\nabla + \tfrac{1}{\omega^2}\mathbf{a}\left(\tfrac{\mathbf{x}}{\lambda},\omega t\right)^2 + V(\mathbf{x}) \end{aligned} \tag{4.12}$$

and

$$\mathcal{D}(W_\lambda(t)) = \left\{\psi \in L^2(\mathbb{R}^d) : W_\lambda(t)\psi \in L^2(\mathbb{R}^d)\right\}. \tag{4.13}$$

The analogous operator in dipole approximation is

$$W_\infty(t) : L^2(\mathbb{R}^d) \supseteq \mathcal{D}(W_\infty(t)) \longrightarrow L^2(\mathbb{R}^d),$$

where

$$W_\infty(\mathbf{x},t) = \tfrac{2i}{\omega}\mathbf{a}\left(0,\omega t\right)\cdot\nabla + \tfrac{1}{\omega^2}\mathbf{a}\left(0,\omega t\right)^2 + V(\mathbf{x}) \tag{4.14}$$

and the domain $\mathcal{D}(W_\infty(t))$ is defined analogously to (4.13). Then

$$H_\lambda(t) = -\Delta + W_\lambda(t) \tag{4.15}$$

and

$$H_\infty(t) = -\Delta + W_\infty(t). \tag{4.16}$$

Lemma 4.4. *$W_\lambda(t)$ is symmetric and relatively $-\Delta$-bounded with $-\Delta$-bound < 1.*

Lemma 4.4 assures that the assumptions of the Kato-Rellich Theorem (Theorem 3.8) are fulfilled, hence assertion (1a) follows.

Proof of Lemma 4.4. Let $W(t) \in \left\{W_\lambda(t), W_\infty(t)\right\}$. In general,

$$\mathcal{D}(W(t)) \not\supseteq \mathcal{D}(-\Delta) = H^2(\mathbb{R}^d),$$

hence we cannot show the relative $-\Delta$-boundedness of $W(t)$ immediately. Instead, we prove that both $\mathcal{C}_c^\infty(\mathbb{R}^d) \subseteq H^2(\mathbb{R}^d)$ and $\mathcal{C}_c^\infty(\mathbb{R}^d) \subseteq \mathcal{D}(W(t))$, then show that $W(t) << -\Delta$ on $\mathcal{C}_c^\infty(\mathbb{R}^d)$, and finally extend $W(t)$ to a $-\Delta$-bounded operator on $H^2(\mathbb{R}^d)$.

By Lemma 3.21, $\mathcal{C}_c^\infty(\mathbb{R}^d) \subseteq H^2(\mathbb{R}^d)$. Further, let $\psi \in \mathcal{C}_c^\infty(\mathbb{R}^d)$. Then by assumption (A4),

$$\begin{aligned} \|W(t)\psi\| &= \left\|\tfrac{2i}{\omega}\mathbf{a}(t)\cdot\nabla\psi + \tfrac{1}{\omega^2}\mathbf{a}(t)^2\psi + V\psi\right\| \\ &\le C\left(\|\nabla\psi\| + \|\psi\|\right) + \|V\psi\|, \end{aligned} \tag{4.17}$$

where $\mathbf{a}(t) \in \left\{\mathbf{a}\left(\tfrac{\cdot}{\lambda},\omega t\right), \mathbf{a}\left(0,\omega t\right)\right\}$, respectively. As $\mathcal{C}_c^\infty(\mathbb{R}^d) \subseteq H^2(\mathbb{R}^d)$, we know from Corollary 3.20 that

$$C\left(\|\nabla\psi\| + \|\psi\|\right) \le C\,\|\psi\|_{H^2(\mathbb{R}^d)} < \infty.$$

The last summand in (4.17) can be written as

$$\|V\psi\| = \left(\int\limits_{\mathrm{supp}(\psi)} |V(\mathbf{x})|^2 |\psi(\mathbf{x})|^2 d\mathbf{x} \right)^{\frac{1}{2}}.$$

Since $|\psi|^2$ is continuous and has compact support, we conclude that it must be bounded, i.e. that there exists some $C < \infty$ such that $|\psi(\mathbf{x})|^2 < C$ for every $\mathbf{x} \in \mathbb{R}^d$. As a consequence,

$$\|V\psi\| < \infty$$

as $V \in L^2_{\mathrm{loc}}(\mathbb{R}^d)$. In conclusion,

$$\|W(t)\psi\| < \infty,$$

and consequently $\psi \in \mathcal{D}(W(t))$, implying $\mathcal{C}_c^\infty(\mathbb{R}^d) \subseteq \mathcal{D}(W(t))$.

The next step is to show that $W(t)$ is symmetric on $\mathcal{C}_c^\infty(\mathbb{R}^d)$. Let $\psi, \varphi \in \mathcal{C}_c^\infty(\mathbb{R}^d)$. Then

$$\langle W(t)\psi, \varphi\rangle = -\tfrac{2i}{\omega} \langle \mathbf{a}(t) \cdot \nabla\psi, \varphi\rangle + \tfrac{1}{\omega^2} \left\langle \mathbf{a}(t)^2\psi, \varphi\right\rangle + \langle V\psi, \varphi\rangle.$$

We integrate the first term by parts, using assumption (A3) and the fact that the boundary terms vanish because ψ and φ are compactly supported. With $\mathbf{a}(t)$ and V being real-valued, this yields

$$\langle W(t)\psi, \varphi\rangle = \langle \psi, W(t)\varphi\rangle,$$

hence $W(t)$ is symmetric on $\mathcal{C}_c^\infty(\mathbb{R}^d)$.

Now we prove the infinitesimal $-\Delta$-boundedness of $W(t)$ on $\mathcal{C}_c^\infty(\mathbb{R}^d)$. The only condition remaining to be verified is assumption (ii) in Definition 3.6.
Let $\psi \in \mathcal{C}_c^\infty(\mathbb{R}^d)$. Then

$$\begin{aligned}\|W(t)\psi\| &\le \tfrac{2}{\omega} \|\mathbf{a}(t) \cdot \nabla\psi\| + \tfrac{1}{\omega^2} \left\|\mathbf{a}(t)^2\psi\right\| + \|V\psi\| \\ &\le C\left(\|\nabla\psi\| + \|\psi\| + \|V\psi\|\right)\end{aligned}$$

independently of t, where we have used the Cauchy-Schwarz inequality in the Euclidean scalar product and the fact that $\|\mathbf{a}(t)\|_\infty \le C$ uniformly in t by assumption (A4). Assumption (A1) gives

$$\|V\psi\| \le \varepsilon \|-\Delta\psi\| + C_\varepsilon \|\psi\|,$$

where $\varepsilon, C_\varepsilon \in \mathbb{R}$ such that

$$\inf\{\varepsilon : \|V\psi\| \le \varepsilon \|-\Delta\psi\| + C_\varepsilon \|\psi\|\} = 0. \tag{4.18}$$

Hence

$$\|W(t)\psi\| \le C\Big(\|\nabla\psi\| + (C_\varepsilon + 1)\|\psi\| + \varepsilon \|-\Delta\psi\| \Big).$$

Furthermore,

$$\begin{aligned}\|\nabla\psi\| &= \left(\sum_{i=1}^d \|\partial_i\psi\|^2\right)^{\frac{1}{2}} = \left(\sum_{i=1}^d \left\langle\psi, (-\partial_i^2)\psi\right\rangle\right)^{\frac{1}{2}} = \langle\psi, (-\Delta)\psi\rangle^{\frac{1}{2}} \\ &\le \left(\tfrac{1}{\varepsilon}\|\psi\|\right)^{\frac{1}{2}} \cdot \left(\varepsilon\|-\Delta\psi\|\right)^{\frac{1}{2}}\end{aligned}$$

due to the CAUCHY-SCHWARZ inequality and the linearity of the scalar product. In the second step we have performed an integration by parts where the boundary terms vanish as $\psi, \varphi \in \mathcal{C}_c^\infty(\mathbb{R}^d)$. With the estimate

$$cd \leq 2cd \leq c^2 + d^2 \tag{4.19}$$

for $c, d \geq 0$ as a corollary from the second binomial formula, we obtain

$$\|\nabla\psi\| \leq \tfrac{1}{2\varepsilon}\|\psi\| + \tfrac{\varepsilon}{2}\|-\Delta\psi\|. \tag{4.20}$$

Altogether,

$$\|W(t)\psi\| \leq \tfrac{C\varepsilon}{2}\|-\Delta\psi\| + C\big(1 + C_\varepsilon + \tfrac{1}{2\varepsilon}\big)\|\psi\|, \tag{4.21}$$

i.e. there exist $\widetilde{\varepsilon}, \widetilde{C_\varepsilon} \in \mathbb{R}$ such that

$$\|W(t)\psi\| \leq \widetilde{\varepsilon}\|-\Delta\psi\| + \widetilde{C_\varepsilon}\|\psi\| \quad \forall\, \psi \in \mathcal{C}_c^\infty(\mathbb{R}^d) \tag{4.22}$$

independently of t. From (4.18) and (4.21) it follows that the infimum of the $\widetilde{\varepsilon}$ is zero, hence $W(t)$ has relative $-\Delta$-bound zero on $\mathcal{C}_c^\infty(\mathbb{R}^d)$ for all $t \in [0, T]$.

Finally, we extend $W(t)$ to an operator from $H^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$. Let $\psi \in H^2(\mathbb{R}^d)$. By density of $\mathcal{C}_c^\infty(\mathbb{R}^d)$ in $H^2(\mathbb{R}^d)$ (Lemma 3.21), there is a sequence $\{\psi_k\}_{k\in\mathbb{N}} \subseteq \mathcal{C}_c^\infty(\mathbb{R}^d)$ such that $\lim_{k\to\infty}\psi_k = \psi$ in $H^2(\mathbb{R}^d)$-norm, which also implies the convergence in $L^2(\mathbb{R}^d)$-norm by Corollary 3.20. By (4.22),

$$\|W(t)\psi_k\| \leq \widetilde{\varepsilon}\|-\Delta\psi_k\| + \widetilde{C_\varepsilon}\|\psi_k\| \quad \forall\psi_k \in \mathcal{C}_c^\infty(\mathbb{R}^d)$$

for $\widetilde{\varepsilon}$ and $\widetilde{C_\varepsilon}$ as above. Define the extension

$$\begin{aligned} W(t) : H^2(\mathbb{R}^d) &\longrightarrow L^2(\mathbb{R}^d) \\ \psi &\longmapsto W(t)\psi = \lim_{k\to\infty} W(t)\psi_k, \end{aligned}$$

where the limit is taken in $L^2(\mathbb{R}^d)$-sense. By continuity of the norm,

$$\begin{aligned} \|W(t)\psi\| &= \lim_{k\to\infty}\|W(t)\psi_k\| \leq \lim_{k\to\infty}\Big(\widetilde{\varepsilon}\|-\Delta\psi_k\| + \widetilde{C_\varepsilon}\|\psi_k\|\Big) \\ &= \widetilde{\varepsilon}\|-\Delta\psi\| + \widetilde{C_\varepsilon}\|\psi\| < \infty \quad \forall\psi \in H^2(\mathbb{R}^d). \end{aligned} \tag{4.23}$$

Thus the limit $W(t)\psi$ exists in $L^2(\mathbb{R}^d)$ and $W(t) << -\Delta$ uniformly in t on $H^2(\mathbb{R}^d)$. The extension is independent of the approximating sequence:
Let $\{\widetilde{\psi}_l\}_{l\in\mathbb{N}} \subseteq \mathcal{C}_c^\infty(\mathbb{R}^d)$ be another approximating subsequence for ψ in $H^2(\mathbb{R}^d)$-sense. Then

$$\Big\|W(t)\psi_k - W(t)\widetilde{\psi}_l\Big\| \leq \widetilde{\varepsilon}\Big\|-\Delta(\psi_k - \widetilde{\psi}_l)\Big\| + \widetilde{C_\varepsilon}\Big\|\psi_k - \widetilde{\psi}_l\Big\| \leq C\Big\|\psi_k - \widetilde{\psi}_l\Big\|_{H^2(\mathbb{R}^d)},$$

and by continuity of the $H^2(\mathbb{R}^d)$-norm,

$$\lim_{k,l\to\infty}\Big\|W(t)\psi_k - W(t)\widetilde{\psi}_l\Big\| \leq C\Big\|\lim_{k\to\infty}\psi_k - \lim_{l\to\infty}\widetilde{\psi}_l\Big\|_{H^2(\mathbb{R}^d)} = 0,$$

as both sequences are approximating ψ in $H^2(\mathbb{R}^d)$-norm. Thus the extension is well-defined. □

In chapter 6, we will quantify the convergence we are currently proving, and as part of this be concerned about the explicit values of the constants $\widetilde{\varepsilon}$ and $\widetilde{C_\varepsilon}$. To this end, define the constant $C_{\mathbf{a}}$ by

$$C_{\mathbf{a}} := \max\left\{ \sup_{t\in[0,T]} \|\mathbf{a}(\cdot,t)\|_\infty \,, \sup_{t\in[0,T]} \|\partial_t \mathbf{a}(\cdot,t)\|_\infty \right\}. \tag{4.24}$$

Reconsidering the argument that led to (4.21) while regarding the explicit values of the constants yields

$$\widetilde{\varepsilon} = \left(1 + \tfrac{1}{\omega} C_{\mathbf{a}}\right) \varepsilon \tag{4.25}$$

and

$$\widetilde{C_\varepsilon} = \tfrac{1}{\omega^2} C_{\mathbf{a}}^2 + \tfrac{1}{\omega\varepsilon} C_{\mathbf{a}} + C_\varepsilon, \tag{4.26}$$

where ε and C_ε are the coefficients of relative boundedness of V.

4.2.2 Uniform Equivalence of Graph Norm and Sobolev Norm

Before expanding on assertions (1b) to (1d), we show an auxiliary lemma which will prove useful at several points. The idea for this lemma is due to [12, 13], the proof differs.

Lemma 4.5. *Let $t \in [0,T]$ and $H(t) \in \{H_\infty(t), H_\lambda(t)\}$. Then the graph norm of $H(t)$ is equivalent to the $H^2(\mathbb{R}^d)$-norm uniformly in t, i.e. $\exists\, C_1, C_2 \geq 0$ such that*

$$\|\psi\|_{H(t)} \leq C_1 \|\psi\|_{H^2(\mathbb{R}^d)} \quad \textit{and} \quad \|\psi\|_{H^2(\mathbb{R}^d)} \leq C_2 \|\psi\|_{H(t)}$$

for each $\psi \in H^2(\mathbb{R}^d)$.

Proof. Let $t \in [0,T]$ and $\psi \in H^2(\mathbb{R}^d)$. By the triangle inequality,

$$\|\psi\|_{H(t)} = \|\psi\| + \|H(t)\psi\| \leq \|\psi\| + \|{-\Delta\psi}\| + \|W(t)\psi\|\,,$$

where $W(t) \in \{W_\lambda(\cdot,t), W_\infty(\cdot,t)\}$. Due to the infinitesimal $-\Delta$-boundedness of $W(t)$ established in (4.23) and as a consequence of Corollary 3.20, we conclude that

$$\|\psi\|_{H(t)} \leq (1 + \widetilde{\varepsilon}\,) \|{-\Delta\psi}\| + (1 + \widetilde{C_\varepsilon}) \|\psi\| \tag{4.27}$$

uniformly in t, hence C_1 is given as

$$C_1 = 1 + \widetilde{\varepsilon} + \widetilde{C_\varepsilon}, \tag{4.28}$$

with $\widetilde{\varepsilon}$ and $\widetilde{C_\varepsilon}$ as in (4.25) and (4.26).

Conversely,

$$\|H(t)\psi\| \geq \|{-\Delta\psi}\| - \|W(t)\psi\| \geq (1 - \widetilde{\varepsilon}\,) \|{-\Delta\psi}\| - \widetilde{C_\varepsilon} \|\psi\|\,,$$

hence

$$\|{-\Delta\psi}\| \leq C \|\psi\|_{H(t)}$$

uniformly in t. Together with estimate (4.20), this implies

$$\|\nabla\psi\| \leq C(\|\psi\| + \|-\Delta\psi\|) \leq C\,\|\psi\|_{H(t)}\,,$$

and as obviously

$$\|\psi\| \leq \|\psi\|_{H(t)}\,,$$

we conclude that

$$\|\psi\|_{H^2(\mathbb{R}^d)} \leq C_2\,\|\psi\|_{H(t)} \tag{4.29}$$

due to Corollary 3.20. Explicit bookkeeping of the constants yields

$$\begin{aligned}
\|\psi\|^2_{H^2(\mathbb{R}^d)} &\leq \|\psi\|^2 + 2(\tfrac{1}{2\varepsilon}\,\|\psi\| + \tfrac{\varepsilon}{2}\,\|-\Delta\psi\|)^2 + \|-\Delta\psi\|^2 \\
&\leq \Big(\big(1+\tfrac{1}{\varepsilon}\big)\,\|\psi\| + (1+\varepsilon)\,\|-\Delta\psi\|\Big)^2 \\
&\leq (\|\psi\| + \|-\Delta\psi\|)^2\big(1+\tfrac{1}{\varepsilon}+\varepsilon\big)^2,
\end{aligned}$$

and together with

$$\|-\Delta\psi\| \leq \frac{\widetilde{C_\varepsilon}}{1-\widetilde{\varepsilon}}\,\|\psi\| + \frac{1}{1-\widetilde{\varepsilon}}\,\|H(t)\psi\|\,, \tag{4.30}$$

we see that the constant C_2 in (4.29) is determined by

$$C_2 = \left(1 + \frac{1}{\varepsilon} + \varepsilon\right)\frac{\widetilde{C_\varepsilon}+1}{1-\widetilde{\varepsilon}}. \tag{4.31}$$

□

Now we proceed to the proof of the remaining parts of Theorem 4.1. In contrast to Sections 4.2.1 and 4.2.2, this represents entirely our own work.

4.2.3 Existence, Uniqueness and Unitarity of the Time Evolutions and Invariance of the Domain

In this section, we prove parts (1b) and (1d) of Theorem 4.1. To this end, we need to show that the assumptions of Theorem 3.38 are satisfied under the identification

$$\begin{aligned}
X &\equiv \Big(L^2(\mathbb{R}^d), \|\cdot\|\Big)\,, \\
Y &\equiv \Big(H^2(\mathbb{R}^d), \|\cdot\|_{H^2(\mathbb{R}^d)}\Big)\,, \\
A(t) &\equiv iH(t),
\end{aligned}$$

where as above $H(t) \in \{H_\infty(t), H_\lambda(t)\}$.

The first step is to show that $iH(t) \in \mathcal{G}(L^2(\mathbb{R}^d))$ for every $t \in [0,T]$. This can easily be seen from the fact that $H(t)$ is self-adjoint as an operator on $L^2(\mathbb{R}^d)$ by assertion (1a). Hence by Stone's Theorem (Theorem 3.32), $iH(t)$ generates a unitary strongly continuous one-parameter group $\{e^{iH(t)s}\}_{s\in\mathbb{R}}$ on $L^2(\mathbb{R}^d)$, which yields a contraction semigroup on $L^2(\mathbb{R}^d)$ if the parameter s varies only within $\mathbb{R}_0^+$. In conclusion, $iH(t) \in \mathcal{G}(L^2(\mathbb{R}^d),1,0) \subset \mathcal{G}(L^2(\mathbb{R}^d))$.

Further, $L^2(\mathbb{R}^d)$ and $H^2(\mathbb{R}^d)$ are both Hilbert spaces and $H^2(\mathbb{R}^d)$ is dense in $L^2(\mathbb{R}^d)$ (Theorem 3.22). It is moreover continuously embedded in $L^2(\mathbb{R}^d)$ because by Corollary 3.20,

$$\|\psi\|_2 \leq \|\psi\|_{H^2(\mathbb{R}^d)} \quad \forall\, \psi \in H^2(\mathbb{R}^d),$$

hence the inclusion map is continuous.

Assumption (i). By Lemma 3.37, $\{iH(t)\}_{0\leq t\leq T}$ is stable with constants of stability $M = 1$ and $\beta = 0$.

Assumption (ii). According to Lemma 3.40, assumption (ii) is implied by the alternative condition (ii'). In order to verify the latter, we define

$$S(t) := iH(t) + \alpha\mathbb{1} : H^2(\mathbb{R}^d) \longrightarrow L^2(\mathbb{R}^d)$$

for some $0 < \alpha \leq 1$[1]. In the following we will show that this operator fulfils condition (ii'). As $-iH(t)$ generates for each $t \in [0, T]$ a contraction semigroup on $L^2(\mathbb{R}^d)$, it follows that $\alpha \in \rho(-iH(t))$ by the Hille-Yosida theorem (Theorem 3.31). Hence $S(t)$ and its inverse,

$$S(t)^{-1} = R_\alpha(-iH(t)) : L^2(\mathbb{R}^d) \longrightarrow H^2(\mathbb{R}^d),$$

are isomorphisms by definition of the resolvent set (Definition 3.12).

Define

$$A_1(t) := S(t)iH(t)S(t)^{-1} : \mathcal{D}(A_1(t)) \longrightarrow L^2(\mathbb{R}^d),$$

where

$$\mathcal{D}(A_1(t)) = \left\{\psi \in L^2(\mathbb{R}^d) : H(t)S(t)^{-1}\psi \in H^2(\mathbb{R}^d)\right\}.$$

If we can show that $-A_1(t)$ is for each $t \in [0, T]$ the generator of a contraction semigroup, we have according to Lemma 3.37 established parts (1) and (2) of condition (ii'), with constants $M_1 = 1$ and $\beta_1 = 0$.
To this end, let $\psi \in L^2(\mathbb{R}^d)$ and $\lambda > 0$. Then

$$\begin{aligned} R_\lambda(-A_1)\psi &= \left[S(t)iH(t)S(t)^{-1} + \lambda\right]^{-1}\psi = \Big(S(t)(iH(t) + \lambda)S(t)^{-1}\Big)^{-1}\psi \\ &= (iH(t) + \alpha)R_\lambda(-iH(t))R_\alpha(-iH(t))\psi, \end{aligned}$$

and as the resolvents of $-iH(t)$ are commutative by Theorem 3.13, we conclude that

$$R_\lambda(-A_1)\psi = (iH(t) + \alpha)R_\alpha(-iH(t))R_\lambda(-iH(t))\psi = R_\lambda(-iH(t))\psi$$

for all $\psi \in L^2(\mathbb{R}^d)$. Thus $(0, \infty) \subseteq \rho(-A_1(t))$ and

$$\|R_\lambda(-A_1(t))\| = \|R_\lambda(-iH(t))\| \leq \frac{1}{\lambda},$$

which by Hille-Yosida proves that $-A_1(t)$ generates a contraction semigroup on $L^2(\mathbb{R}^d)$.

[1] As the resolvent set $\rho(-iH(t))$ contains all positive real numbers it is irrelevant which α we choose, provided it being greater than zero. We choose $\alpha \leq 1$ without loss of generality because this simplifies some estimates later in the proof.

Part (3) of condition (ii') demands that $S(t)$ and $S(t)^{-1}$ be bounded in their respective operator norm by a common constant γ uniformly in t.
First,

$$\begin{aligned}\|S(t)\|_{H^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} &= \sup_{\substack{\psi\in H^2(\mathbb{R}^d)\\ \psi\neq 0}} \frac{\|(iH(t)+\alpha)\psi\|}{\|\psi\|_{H^2(\mathbb{R}^d)}} \\ &\leq \sup_{\substack{\psi\in H^2(\mathbb{R}^d)\\ \psi\neq 0}} \frac{\|H(t)\psi\|+\|\psi\|}{\|\psi\|_{H^2(\mathbb{R}^d)}} = \sup_{\substack{\psi\in H^2(\mathbb{R}^d)\\ \psi\neq 0}} \frac{\|\psi\|_{H(t)}}{\|\psi\|_{H^2(\mathbb{R}^d)}}\end{aligned} \tag{4.32}$$

as $\alpha \leq 1$. Lemma 4.5 yields thus

$$\|S(t)\|_{H^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \leq C_1 < \infty \tag{4.33}$$

uniformly in t, with C_1 as in (4.28). Second,

$$\begin{aligned}\left\|S(t)^{-1}\right\|_{L^2(\mathbb{R}^d)\to H^2(\mathbb{R}^d)} &= \sup_{\substack{\psi\in L^2(\mathbb{R}^d)\\ \psi\neq 0}} \frac{\left\|(iH(t)+\alpha)^{-1}\psi\right\|_{H^2(\mathbb{R}^d)}}{\|\psi\|} \\ &\leq C_2 \sup_{\substack{\psi\in L^2(\mathbb{R}^d)\\ \psi\neq 0}} \left(\frac{\left\|(iH(t)+\alpha)^{-1}\psi\right\|}{\|\psi\|} + \frac{\left\|H(t)(iH(t)+\alpha)^{-1}\psi\right\|}{\|\psi\|}\right)\end{aligned}$$

with C_2 as in (4.31) by Lemma 4.5. The first term can be estimated as

$$\frac{\left\|(iH(t)+\alpha)^{-1}\psi\right\|}{\|\psi\|} \leq \|R_\alpha(-iH(t))\| < \frac{1}{\alpha}$$

due to Hille-Yosida. For the second term, we consider

$$\begin{aligned}\left\|H(t)(iH(t)+\alpha)^{-1}\psi\right\| &= \left\|(iH(t)+\alpha-\alpha)(iH(t)+\alpha)^{-1}\psi\right\| \\ &= \left\|\psi-\alpha(iH(t)+\alpha)^{-1}\psi\right\| \\ &\leq \|\psi\| + \alpha\,\|R_\alpha(-iH(t))\psi\| \leq 2\,\|\psi\|\,.\end{aligned}$$

Hence

$$\left\|S(t)^{-1}\right\|_{L^2(\mathbb{R}^d)\to H^2(\mathbb{R}^d)} \leq C_2\left(\frac{1}{\alpha}+2\right) < \infty \tag{4.34}$$

uniformly in t. (4.33) and (4.34) prove part (3) with

$$\gamma = \max\left\{C_1, (\tfrac{1}{\alpha}+2)C_2\right\}. \tag{4.35}$$

It remains to verify part (4) of condition (ii'), stating that $t \mapsto S(t)$ must be of bounded variation.
Let $0 = t_0 < t_1 < \cdots < t_n = T$ be a partition of $[0, T]$ and let $1 \leq j \leq n$. In the following, the operator norm $\|\cdot\|_{H^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)}$ shall be denoted by $\|\cdot\|_{\mathrm{op}}$. Then

$$\|S(t_j)-S(t_{j-1})\|_{\mathrm{op}} = \|iH(t_j)-iH(t_{j-1})\|_{\mathrm{op}}\,,$$

and

$$\begin{aligned}\|iH(t_j) - iH(t_{j-1})\|_{\text{op}} &\leq \tfrac{2}{\omega} \|(\mathbf{a}(t_j) - \mathbf{a}(t_{j-1})) \cdot \nabla\|_{\text{op}} + \tfrac{1}{\omega^2} \left\|\mathbf{a}(t_j)^2 - \mathbf{a}(t_{j-1})^2\right\|_{\text{op}} \\ &\leq \tfrac{2}{\omega} \|\mathbf{a}(t_j) - \mathbf{a}(t_{j-1})\|_\infty \|\nabla\|_{\text{op}} + \tfrac{1}{\omega^2} \left\|\mathbf{a}(t_j)^2 - \mathbf{a}(t_{j-1})^2\right\|_\infty \|\mathbb{1}\|_{\text{op}} .\end{aligned}$$

By Corollary 3.20, $\|\nabla\psi\|_{\text{op}} \leq \frac{1}{2}$ and $\|\mathbb{1}\|_{\text{op}} \leq 1$, hence

$$\|iH(t_j) - iH(t_{j-1})\|_{\text{op}} \leq \tfrac{1}{\omega} \|\mathbf{a}(t_j) - \mathbf{a}(t_{j-1})\|_\infty + \tfrac{1}{\omega^2} \left\|\mathbf{a}(t_j)^2 - \mathbf{a}(t_{j-1})^2\right\|_\infty . \tag{4.36}$$

Bearing in mind that $\mathbf{a}(t)$ is only an abbreviation for a function depending on $\frac{\mathbf{x}}{\lambda}$ or 0 in the first and on ωt in the second slot, we know that there must exist a $\xi \in (t_{j-1}, t_j)$ such that

$$\|\mathbf{a}(t_j) - \mathbf{a}(t_{j-1})\|_\infty \leq |\omega(t_j - t_{j-1})| \cdot \|\partial_t \mathbf{a}(\xi)\|_\infty \leq \omega C_{\mathbf{a}} |t_j - t_{j-1}| \tag{4.37}$$

by the mean value theorem and assumption (A4). Analogously, we derive that

$$\left\|\mathbf{a}(t_j)^2 - \mathbf{a}(t_{j-1})^2\right\|_\infty \leq \omega C_{\mathbf{a}}^2 |t_j - t_{j-1}|, \tag{4.38}$$

with $C_{\mathbf{a}}$ as in (4.24). Insertion of (4.37) and (4.38) into (4.36) yields

$$\|iH(t_j) - iH(t_{j-1})\|_{\text{op}} \leq C_3 |t_j - t_{j-1}|, \tag{4.39}$$

where

$$C_3 := C_{\mathbf{a}} + \tfrac{1}{\omega} C_{\mathbf{a}}^2. \tag{4.40}$$

Altogether, we obtain

$$\sum_{j=1}^{n} \|S(t_j) - S(t_{j-1})\|_{\text{op}} \leq C_3 \sum_{j=1}^{n} |t_j - t_{j-1}| = C_3 T,$$

which shows that $t \mapsto S(t)$ is of bounded variation. This concludes the proof of condition (ii'). As a consequence, (ii) holds with constants $\widetilde{\beta} = 0$ and $\widetilde{M} = \gamma^2 e^{\gamma C_3 T}$, with γ as in (4.35).

Assumption (iii). From assertion (1a) we already know that $H^2(\mathbb{R}^d) = \mathcal{D}(H(t))$ for all t. Moreover, $iH(t) \in \mathcal{L}(H^2(\mathbb{R}^d), L^2(\mathbb{R}^d))$ for each t, because $S(t) = iH(t) + \alpha$ is bounded as an operator from $H^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$, as established in (4.33).

It remains to show that $t \mapsto iH(t)$ is continuous with respect to $\|\cdot\|_{H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)} \equiv \|\cdot\|_{\text{op}}$. To this end, let $\varepsilon > 0$ and choose $\delta = \frac{\varepsilon}{C_3}$, with C_3 as in (4.40)[2]. Let $t_1, t_2 \in [0, T]$ such that $|t_1 - t_2| < \delta$. Choosing $j = 2$ in (4.39), we obtain

$$\|iH(t_1) - iH(t_2)\|_{\text{op}} \leq C_3 |t_1 - t_2| < C_3 \delta \leq \varepsilon, \tag{4.41}$$

which proves the norm-continuity of $iH(t)$.

Assumptions (i) to (iii) of Theorem 3.38 being fulfilled, this theorem establishes existence and uniqueness of the evolution operator $U(t, t_0) \in \{U_\lambda(t, t_0), U_\infty(t, t_0)\}$ and the invariance of the domain under $U(t, t_0)$ for $t \in [0, T]$. The unitarity of $U(t, t_0)$ follows directly from Theorem 3.45. This concludes the proof of parts (1b) and (1d).

[2] We may restrict our analysis to the case $C_3 \neq 0$ – otherwise, (4.39) would imply $H(t_2)\psi = H(t_1)\psi$ for all $\psi \in H^2(\mathbb{R}^d)$, thus $t \mapsto S(t)$ would be trivially continuous.

4.2.4 Strong Continuity of the Time Evolutions

We come now to the last part of Section 4.2, the proof of assertion (1c). In order to establish the strong continuity of $U(t,t_0)$ jointly in t and t_0, we need to show that the assumptions of Theorem 3.41 are satisfied. Taking into account the results obtained previously, it only remains to prove that also condition (ii") is true for $X \equiv L^2(\mathbb{R}^d)$, $Y \equiv H^2(\mathbb{R}^d)$ and $A(t) \equiv iH(t)$.

One could now raise the question why we have not invoked this more general Theorem 3.41 already in section 4.2.3, although it includes not only assertion (1c) but comprises parts (1b) and (1d) as well. The reason is that we wished to quantify the coefficients of stability $\widetilde{M}$ and $\widetilde{\beta}$, which emerge immediately from the proof of condition (ii').

As above, define $S(t) = iH(t) + \alpha$, where $0 < \alpha \leq 1$. For the differentiability of $S(t)$ it suffices to show that $t \mapsto H(t)$ is differentiable.
Let $\psi \in H^2(\mathbb{R}^d)$, $t \in [0,T]$ and $h \neq 0$. Then

$$\begin{aligned} \tfrac{1}{|h|} \left\| H(t+h)\psi - H(t)\psi \right\| &= \tfrac{1}{|h|} \left\| \big(H(t+h) - H(t)\big)\psi \right\| \\ &\leq \tfrac{1}{|h|} C_3 |(t+h) - t| \left\|\psi\right\| \leq C_3 \left\|\psi\right\| < \infty, \end{aligned} \tag{4.42}$$

and consequently

$$\tfrac{1}{|h|} \left\| H(t+h) - H(t) \right\|_{H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)} \leq C_3$$

by (4.39), with C_3 as in (4.40). Thus the derivative $\partial_t H(t)\psi$ exists and, recalling that $\mathbf{a}(t)$ really depends on ωt in the second slot, can be calculated as

$$\partial_t H(t)\psi = 2i\partial_t \mathbf{a}(t) \cdot \nabla\psi + \tfrac{1}{\omega} \partial_t \mathbf{a}(t)^2 \psi. \tag{4.43}$$

We further need to establish the continuity of this derivative. Let $\varepsilon > 0$ and choose $\delta = \frac{\varepsilon}{C}$ for some appropriately chosen constant $C > 0$. Let $t_1, t_2 \in [0,T]$ such that $|t_1 - t_2| < \delta$. Then

$$\begin{aligned} \left\| \big(\partial_t H(t_1) - \partial_t H(t_2)\big)\psi \right\| &\leq 2 \left\| \big(\partial_t \mathbf{a}(t_1) - \partial_t \mathbf{a}(t_2)\big) \cdot \nabla\psi \right\| + \tfrac{1}{\omega} \left\| (\partial_t \mathbf{a}(t)^2 - \partial_t \mathbf{a}(t)^2)\psi \right\| \\ &\leq \Big(\left\| \partial_t \mathbf{a}(t_1) - \partial_t \mathbf{a}(t_2) \right\|_\infty + \left\| \partial_t \mathbf{a}(t)^2 - \partial_t \mathbf{a}(t)^2 \right\|_\infty \Big) \left\|\psi\right\|, \end{aligned}$$

where we have used that $\|\nabla\|_{H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)} \leq \frac{1}{2}$. With $\mathbf{a}(t)$ being $\mathcal{C}^2$ in t, we may apply the mean value theorem to $\partial_t \mathbf{a}(t)$ and $\partial_t \mathbf{a}(t)^2$ analogously to (4.37) and (4.38). This yields

$$\left\| \big(\partial_t H(t_1) - \partial_t H(t_2)\big)\psi \right\| \leq C|t_1 - t_2| \left\|\psi\right\| < C\delta \left\|\psi\right\| \leq \varepsilon \left\|\psi\right\|, \tag{4.44}$$

and as a consequence

$$\left\| \partial_t H(t_1) - \partial_t H(t_2) \right\|_{H^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)} \leq \varepsilon,$$

which concludes the proof of part (1) of condition (ii").
Parts (2) and (3) follow immediately from the observation that

$$S(t)A(t)S(t)^{-1} = \big(iH(t) + \alpha\big) iH(t) \big(iH(t) + \alpha\big)^{-1} = iH(t) = A(t).$$

Having verified all assumptions of Theorem 3.41, we conclude that $U(t,s)$ is strongly continuous with respect to $\|\cdot\|_{H^2(\mathbb{R}^d)}$ jointly in t and s. The joint continuity with respect to the $L^2(\mathbb{R}^d)$-norm can be deduced from this as follows: due to the joint continuity ($H^2(\mathbb{R}^d)$), we know that for each $\varphi \in H^2(\mathbb{R}^d)$ and $\varepsilon > 0$, there exists $\delta > 0$ such that

$$\left\| \big(U(t_1,s_1) - U(t_2,s_2)\big)\varphi \right\|_{H^2(\mathbb{R}^d)} < \tfrac{\varepsilon}{2} \quad \forall\, |(s_1,t_1) - (s_2,t_2)| < \delta. \tag{4.45}$$

By Corollary 3.20, this implies as well

$$\left\| \big(U(t_1,s_1) - U(t_2,s_2)\big)\varphi \right\| < \tfrac{\varepsilon}{2}. \tag{4.46}$$

Now let $\psi \in L^2(\mathbb{R}^d)$ and $\varepsilon > 0$. Due to the density of $H^2(\mathbb{R}^d)$ in $L^2(\mathbb{R}^d)$ (Theorem 3.22), we can find a $\varphi \in H^2(\mathbb{R}^d)$ such that $\|\psi - \varphi\| < \frac{\varepsilon}{4}$. Choose δ such that (4.45) holds. Then we obtain

$$\begin{aligned} \left\| \big(U(t_1,s_1) - U(t_2,s_2)\big)\psi \right\| &\le \left\| \big(U(t_1,s_1) - U(t_2,s_2)\big)\varphi \right\| + \left\| \big(U(t_1,s_1) - U(t_2,s_2)\big)(\psi - \varphi) \right\| \\ &\le \tfrac{\varepsilon}{2} + 2\,\|\psi - \varphi\| < \varepsilon, \end{aligned}$$

where we have used (4.46) and the fact that $U(t,s)$ is unitary. This finally concludes the proof of Part 1. □

4.3 Proof of Part 1 using Yosida's Theorem

In the following, we will present another way of proving the first part of Theorem 4.1. Instead of applying Kato's theorems, we will show that Theorem 3.42 by Yosida holds true under the identification

$$\begin{aligned} X &\equiv \Big(L^2(\mathbb{R}^d), \|\cdot\|\Big), \\ \mathcal{D} &\equiv \Big(H^2(\mathbb{R}^d), \|\cdot\|_{H^2(\mathbb{R}^d)}\Big), \\ A(t) &\equiv -i(H(t) + \mu\mathbb{1}), \end{aligned}$$

where as above $H(t) \in \{H_\infty(t), H_\lambda(t)\}$. This section is again inspired by [12, 13]. Our proof is however considerably easier because we make use of the work of Griesemer and Schmid (Lemma 3.44) to simplify the verification of condition (iv) of Theorem 3.42.

We choose $\mu > \widetilde{C_\varepsilon}$, with $\widetilde{C_\varepsilon}$ as defined in (4.26). This implies $0 \in \rho(H(t) + \mu)$ because, as a consequence of Theorem 3.10, the spectrum of $H(t)$ is bounded below by $-\widetilde{C_\varepsilon}$. Due to the self-adjointness of $H(t)$, the spectrum is a subset of the real line, hence the spectrum of $H(t) + \mu$ is completely positive.
The new $A(t)$ is very similar to $-S(t)$ from the previous section, hence we can use several of the preceding results. The relative minus sign of $A(t)$ arises because we consider now the evolution equation in the form (3.40) instead of (3.20).

It is important to note that the successful verification of the assumptions of Yosida's theorem does not immediately prove Theorem 4.1, because we are using $A(t) = -i(H(t) + \mu)$ instead of the true generator $-iH(t)$. This is however easily overcome: suppose we have shown that the operator $A(t) = -i(H(t) + \mu)$ generates the time evolution operator $\widetilde{U}(t,s)$. The time evolution operator $U(t,s)$ generated by $-iH(t)$ is then given as

$$U(t,s) = \widetilde{U}(t,s)e^{-i\mu(t-s)}.$$

Hence it suffices to prove the assumptions for $A(t)$ as above.

Assumption (i). We have to show that $\mathcal{D}(A(t))$ is independent of t and dense in $L^2(\mathbb{R}^d)$. This was already shown in section 4.2.1.

Assumption (ii). It needs to be verified that $R_\lambda(A(t))$ is bounded for each $\lambda \geq 0$ and that $\|R_\lambda(A(t))\| \leq \frac{1}{\lambda}$ for $\lambda > 0$. For $\lambda = 0$, the claim is clear because we have chosen μ such that $0 \in \rho(H(t) + \mu)$, and

$$R_0(A(t)) = iR_0(H(t) + \mu),$$

hence $0 \in \rho(A(t))$. For $\lambda > 0$, consider

$$R_\lambda(A(t)) = (\lambda + i\mu + iH(t))^{-1} = R_{\lambda+i\mu}(-iH(t)).$$

As $-iH(t)$ is the generator of a contraction semigroup, the Hille-Yosida theorem (Theorem 3.31c) yields

$$\|R_{\lambda+i\mu}(-iH(t))\| \leq \frac{1}{\lambda}.$$

Assumption (iii). We have to prove that $A(t)A(s)^{-1}$ is a bounded operator. To this end, let $s, t \in [0, T]$ and $\psi \in L^2(\mathbb{R}^d)$. Analogously to the proof of part (3) of condition (ii') ((4.32) to (4.35)), we obtain

$$\begin{aligned}
\left\|A(t)A(s)^{-1}\psi\right\| &= \left\|(H(t) + \mu)(H(s) + \mu)^{-1}\psi\right\| \\
&\leq \|H(t) + \mu\|_{H^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} \left\|(H(s) + \mu)^{-1}\right\|_{L^2(\mathbb{R}^d)\to H^2(\mathbb{R}^d)} \|\psi\| \\
&\leq C_1C_2(1 + \mu)\left(\tfrac{1}{\mu} + 2\right) < \infty
\end{aligned}$$

as $\mu \in \rho(-H(s))$. This proves assumption (iii).

Assumption (iv). Instead of proving the assumption directly, we use Lemma 3.44 and show the more straightforward condition (iv'). Obviously, $t \mapsto A(t)\psi = -i(H(t) + \mu))\psi$ is continuously differentiable precisely if $t \mapsto H(t)$ is continuously differentiable. This was already established in (4.44), hence the proof is complete. $\square$

4.4 Estimate of the Kinetic Energy

Before moving on to Part 2, we estimate the kinetic energy of the system. We begin with a general estimate (Lemma 4.6), which we then improve for the case of the wave function evolving under $U_\infty(t, t_0)$ (Lemma 4.8).

Both estimates concern only $H^2(\mathbb{R}^d)$-functions and are not true for generic elements of $L^2(\mathbb{R}^d)$. This does however not pose any problems; it is connected to the fact that $L^2(\mathbb{R}^d)$ contains by construction *unphysical* states, in the sense that they do not occur in nature. Although the time evolution is defined on the whole Hilbert space, not any $L^2(\mathbb{R}^d)$-function is sensible as an initial condition of the Schrödinger equation[3] as it does not necessarily lie within the domain of the Hamiltonian (in other words, it needs not be differentiable). The reason why we work with the whole space $L^2(\mathbb{R}^d)$ and not only with the subspace of *physical* states is simple: we need a complete Hilbert space of square integrable functions to use concepts such as self-adjointness and limits of sequences. Hence the *unphysical* states are merely limiting points of physical states, which are included in the description for reasons of convenience [46, 24, 25].

With $L^2(\mathbb{R}^d)$ containing functions with infinitely large kinetic energy, there is by all means no sense in trying to find an estimate for these states. Hence it is no restriction that our results apply merely to $H^2(\mathbb{R}^d)$-functions.

4.4.1 A First Estimate

In this section, we will apply the abbreviation

$$\psi_t \equiv U(t,t_0)\psi, \tag{4.47}$$

where $U(t,t_0) \in \{U_\lambda(t,t_0), U_\infty(t,t_0)\}$. Obviously this implies $\psi_{t_0} = \psi$, and in this case we will drop the subscript.

Lemma 4.6. *Let $\psi \in H^2(\mathbb{R}^d)$. Then*

$$\|\psi_t\|_{H^2(\mathbb{R}^d)} \leq C \|\psi\|_{H^2(\mathbb{R}^d)} e^{\widetilde{C}t}$$

for some constants $C, \widetilde{C} < \infty$.

Proof. Let $\varphi, \psi \in H^2(\mathbb{R}^d)$ and define $\varphi_t \equiv U(t,t_0)\varphi$ analogously to (4.47). By the fundamental theorem of calculus, we obtain

$$\begin{aligned}
\langle \varphi_t, H(t)\psi_t\rangle &= \langle \varphi_t, H(t)\psi_t\rangle\big|_{t=t_0} + \int_{t_0}^{t} \partial_s \langle \varphi_s, H(s)\psi_s\rangle \, ds \\
&= \langle \varphi, H(t_0)\psi\rangle + \int_{t_0}^{t} \Big(\langle(\partial_s\varphi_s), H(s)\psi_s\rangle + \langle \varphi_s, (\partial_s H(s))\psi_s\rangle + \langle H(s)\varphi_s, (\partial_s\psi_s)\rangle\Big) ds \\
&= \langle \varphi, H(t_0)\psi\rangle + \int_{t_0}^{t} \big\langle \varphi_s, \big(\partial_s H(s)\big)\psi_s\big\rangle \, ds,
\end{aligned}$$

[3] This is true if we are interested in solutions in $L^2(\mathbb{R}^d)$-sense. With a weaker definition of the notion of a solution, it is possible to make sense of $L^2(\mathbb{R}^d)$-functions solving the Schrödinger equation *in the sense of distributions.* If one is however interested in *classical* solutions, the space $H^2(\mathbb{R}^d)$ is still too large. A detailed analysis can be found in [46, 47].

where the last step is an application of the Schrödinger equation. We can rewrite this as

$$\left\langle \varphi, U(t,t_0)^\dagger H(t)\psi_t \right\rangle = \left\langle \varphi, \left(H(t_0)\psi + \int_{t_0}^{t} U(s,t_0)^\dagger \big(\partial_s H(s)\big)\psi_s \, ds \right) \right\rangle \tag{4.48}$$

for each $\varphi \in H^2(\mathbb{R}^d)$. Our next step will be to conclude from (4.48) that

$$\left\| U(t,t_0)^\dagger H(t)\psi_t \right\| = \left\| H(t_0)\psi + \int_{t_0}^{t} U(s,t_0)^\dagger \big(\partial_s H(s)\big)\psi_s \, ds \right\|. \tag{4.49}$$

We need to show that for $\psi_1, \psi_2 \in L^2(\mathbb{R}^d)$, $\langle \phi, \psi_1 \rangle = \langle \phi, \psi_2 \rangle \ \forall \phi \in H^2(\mathbb{R}^d)$ implies that $\|\psi_1\| = \|\psi_2\|$. The statement would be clear if ϕ was an arbitrary element of $L^2(\mathbb{R}^d)$ instead of $H^2(\mathbb{R}^d)$. We thus apply a density argument: let $\phi \in L^2(\mathbb{R}^d)$. By density, we can find a sequence $\{\phi_n\}_{n\in\mathbb{N}} \subseteq H^2(\mathbb{R}^d)$ such that $\|\phi - \phi_n\| \le \frac{1}{n}$, and consequently $\|\phi_n\| \le 1 + \|\phi\|$. Hence

$$\langle \phi, (\psi_1 - \psi_2) \rangle = \lim_{n\to\infty} \langle \phi_n, (\psi_1 - \psi_2) \rangle = 0,$$

as each $\phi_n \in H^2(\mathbb{R}^d)$. We may interchange scalar product and limit as a consequence of the theorem of dominated convergence, because

$$\langle \phi_n, (\psi_1 - \psi_2) \rangle \le (1 + \|\phi\|) \, \|\psi_1 - \psi_2\|$$

is bounded uniformly in n. Thus (4.49) holds true.

With (4.49) and the unitarity of $U(s,t_0)$, we conclude

$$\|H(t)\psi_t\| \le \|H(t_0)\psi\| + \int_{t_0}^{t} \left\| \big(\partial_s H(s)\big)\psi_s \right\| ds. \tag{4.50}$$

Now (4.43) and assumption (A4) yield

$$\begin{aligned} \left\| \big(\partial_s H(s)\big)\psi_s \right\| &\le 2C_{\mathbf{a}} \, \|\nabla\psi_s\| + \tfrac{1}{\omega} C_{\mathbf{a}}^2 \, \|\psi_s\| \\ &\le C_3 \, \|\psi_s\|_{H^2(\mathbb{R}^d)} \le C_2 C_3 \, \|\psi_s\|_{H(s)} \, , \end{aligned} \tag{4.51}$$

with C_2 and C_3 defined as in (4.31) and (4.40), respectively. Inserting (4.51) into (4.50), we finally obtain

$$\|H(t)\psi_t\| \le \|H_{t_0}\psi\| + C_2 C_3 \int_{t_0}^{t} \left(\|H(s)\psi_s\| + \|\psi\| \right) ds.$$

Now we can apply the GRONWALL-BELLMAN inequality (Theorem 3.47) under the identification

$$\begin{aligned} u(t) &\equiv \|H(t)\psi_t\| + \|\psi\| \, , \\ c &\equiv \|H(t_0)\psi\| + \|\psi\| \, , \\ f(s) &\equiv C_2 C_3, \\ [\alpha, \beta] &\equiv [t_0, t]. \end{aligned}$$

The assumptions of Theorem 3.47 are obviously fulfilled, hence

$$\begin{aligned}\|H(t)\psi_t\| + \|\psi_t\| &\leq (\|H(t_0)\psi\| + \|\psi\|) \exp\left\{\int_{t_0}^{t} C_2 C_3 ds\right\} \\ &= (\|H(t_0)\psi\| + \|\psi\|) e^{C_2 C_3 (t-t_0)}.\end{aligned}$$

Therefore we conclude

$$\|\psi_t\|_{H(t)} \leq \|\psi\|_{H(t_0)} \, e^{C_2 C_3 (t-t_0)}, \tag{4.52}$$

which implies

$$\begin{aligned}\|\psi_t\|_{H^2(\mathbb{R}^d)} &\leq C_2 \|\psi_t\|_{H(t)} \leq C_2 \|\psi\|_{H(t_0)} \, e^{C_2 C_3 (t-t_0)} \\ &\leq C_1 C_2 \|\psi\|_{H^2(\mathbb{R}^d)} \, e^{C_2 C_3 (t-t_0)}.\end{aligned}$$

This proves the lemma. □

Together with Corollary 3.20, Lemma 4.6 implies that

$$\|\nabla\psi_t\| \leq C_2 \left(\|\psi\| + \|H(t_0)\psi\|\right) e^{C_2 C_3 (t-t_0)},$$

$$\|-\Delta\psi_t\| \leq C_2 \left(\|\psi\| + \|H(t_0)\psi\|\right) e^{C_2 C_3 (t-t_0)}$$

for $\psi \in H^2(\mathbb{R}^d)$. The first statement yields the desired estimate for the kinetic energy,

$$\|\nabla\psi_t\|^2 \leq C_2^2 \left(\|\psi\| + \|H(t_0)\psi\|\right)^2 e^{2C_2 C_3 (t-t_0)}, \tag{4.53}$$

i.e. the kinetic energy grows at most exponentially in time.

Lemma 4.6 can as well be proved directly from assertion (e) of Kato's Theorem 3.38. An indirect way via Lemma 3.43 from the proof of Yosida's theorem 3.42 can be found in [12, 13]. We have chosen to present the proof in the actual form because it argues directly from the Schrödinger equation, which seems more intuitive than the use of abstract theorems.

4.4.2 An Improved Estimate for the Time Evolution in Dipole Approximation

The Hamiltonian in dipole approximation exhibits a feature which greatly simplifies most calculations: $H_\infty(t_1)$ and $H_\infty(t_2)$ at different instants of time t_1 and t_2 commute, and as a consequence, $H_\infty(t)$ commutes with the time evolution it generates. Whereas this behaviour is immediately clear for time-independent Hamiltonians due to their virtue as generators of contraction semigroups (Theorem 3.29), it is a priori not given in the time-dependent case. It is certainly not true for the exact Hamiltonian $H_\lambda(t)$. We phrase this result in form of a lemma.

Lemma 4.7. *Let $t, t_0, s \in [0, T]$, $t_0 \leq s$, and $H_\infty(t)$ and $U_\infty(t, t_0)$ as in Theorem 4.1. Then*

$$\big[H_\infty(t), U_\infty(s, t_0)\big]\psi = 0$$

for all $\psi \in H^2(\mathbb{R}^d)$.

Proof. We recall the construction of $U_\infty(t,t_0)$ in Theorems 3.38 and 3.42: the time interval $[0,T]$ is partitioned into n smaller intervals on which the Hamiltonian is kept constant and the time evolution thus given by STONE's theorem. We obtain an approximating operator $U_n(t,s)$ by concatenating the time evolution operators over each of the intervals in accordance with the semigroup property. The true time evolution arises from the limiting case $n\to\infty$, when the width of the small intervals tends to zero.

Let $n\in\mathbb{N}$. We can express $U_n(s,t_0)$ as

$$U_n(s,t_0)=e^{-i(s-r_1)H_\infty(r_1)}\cdots e^{-i(r_k-t_0)H_\infty(r_k)}, \tag{4.54}$$

where $r_1,\dots,r_k$, $k\le n$, are the borders of said small intervals of the partition[4]. According to Definition 3.14, two operators commute if and only if their spectral projections commute. Since $[H_\infty(r),H_\infty(t)]=0$, the spectral theorem yields

$$\left[e^{iuH_\infty(r)},H_\infty(t)\right]=0$$

for any $t,u,r\in[0,T]$. We thus conclude that $H_\infty(t)$ commutes with each factor in (4.54), and as a consequence,

$$U_n(s,t_0)H_\infty(t)\psi=H_\infty(t)U_n(s,t_0)\psi \tag{4.55}$$

for each $\psi\in H^2(\mathbb{R}^d)$. The claim of the lemma follows immediately if we can show that the theorem of dominated convergence applies to

$$\|H_\infty(t)U_n(s,t_0)\psi-U_n(s,t_0)H_\infty(t)\psi\|\,. \tag{4.56}$$

This can easily be seen: using (4.55) and the unitarity of $U_n(s,t_0)$, we estimate

$$\begin{aligned}\|H_\infty(t)U_n(s,t_0)\psi-U_n(s,t_0)H_\infty(t)\psi\| &\le \|H_\infty(t)U_n(s,t_0)\psi\|+\|U_n(s,t_0)H_\infty(t)\psi\|\\ &=2\,\|H_\infty(t)\psi\|\le C\,\|\psi\|_{H^2(\mathbb{R}^d)}\end{aligned}$$

according to Lemma 4.5, hence we may interchange limit and norm. This concludes the proof. □

This result enables us to improve the estimate for the kinetic energy when applying the dipole approximation. In order to keep notation simple, we define a new abbreviation: from now on, ψ_t^∞ denotes a wave function evolving according to the approximated Hamiltonian,

$$\psi_t^\infty\equiv U_\infty(t,t_0)\psi. \tag{4.57}$$

Lemma 4.8. *Let $t_0,t\in[0,T]$, $t_0\le t$, and $\psi\in H^2(\mathbb{R}^d)$. With $H_\infty(t)$ and $U_\infty(t,t_0)$ as in Theorem 4.1, it holds that*

$$\|\nabla\psi_t^\infty\|^2\le C\left(\|\nabla\psi\|^2+\|\psi\|^2\right) \tag{4.58}$$

and

$$\|-\Delta\psi_t^\infty\|^2\le\widetilde{C}\left(\|-\Delta\psi\|^2+\|\psi\|^2\right) \tag{4.59}$$

for some constants $C,\widetilde{C}>0$, which are in particular independent of t.

[4] To be exact, we put $r_1:=\frac{T}{n}\left[\frac{ns}{T}\right],\dots,r_k:=\frac{T}{n}\left(\left[\frac{nt_0}{T}\right]+1\right)$.

In other words, there exists a constant C such that

$$\|\psi_t^\infty\|_{H^2(\mathbb{R}^d)} \leq C\,\|\psi\|_{H^2(\mathbb{R}^d)}\,.$$

Proof. In the proof of Lemma 4.4, we have already established in (4.23) that $W(t) << -\Delta$ uniformly in t. Using the equivalent condition (3.2) for infinitesimal boundedness from Lemma 3.7, we conclude that there are constants $\varepsilon', C'_\varepsilon > 0$ such that

$$\|W_\infty(t)\varphi\|^2 \leq \varepsilon'^2\,\|-\Delta\varphi\|^2 + C'^2_\varepsilon\,\|\varphi\|^2$$

for all $\varphi \in H^2(\mathbb{R}^d)$ independent of t. ε' and C'_ε are related to $\widetilde{\varepsilon}$ and $\widetilde{C_\varepsilon}$ as in the proof of Lemma 3.7. Since $-\Delta$ and $\mathbb{1}$ are positive operators, we obtain

$$\|W_\infty(t)\varphi\|^2 \leq \left\|\left(-\varepsilon'\Delta + C'_\varepsilon\right)\varphi\right\|^2,$$

hence the conditions of the HEINZ inequality (Lemma 3.11) are fulfilled. As a consequence, we obtain

$$\begin{aligned} |\langle\varphi, W_\infty(t)\varphi\rangle| &\leq \left\langle\varphi, \left(-\,\varepsilon'\Delta + C'_\varepsilon\right)\varphi\right\rangle \\ &= \varepsilon'\,\langle\varphi, -\Delta\varphi\rangle + C'_\varepsilon\,\|\varphi\|^2 \end{aligned}$$

and thus

$$|\langle\varphi, H_\infty(t)\varphi\rangle| \leq (1+\varepsilon')\,\langle\varphi, -\Delta\varphi\rangle + C'_\varepsilon\,\|\varphi\|^2 \tag{4.60}$$

for all $\varphi \in H^2(\mathbb{R}^d)$ and $t \in [0,T]$. Moreover, we estimate

$$\begin{aligned} |\langle\varphi, H_\infty(t)\varphi\rangle| &\geq \langle\varphi, -\Delta\varphi\rangle - |\langle\varphi, W_\infty(t)\varphi\rangle| \\ &\geq (1-\varepsilon')\,\langle\varphi, -\Delta\varphi\rangle - C'_\varepsilon\,\|\varphi\|^2\,. \end{aligned}$$

This leads to

$$\langle\varphi, -\Delta\varphi\rangle \leq (1-\varepsilon')^{-1}\left(|\langle\varphi, H_\infty(t)\varphi\rangle| + C'_\varepsilon\,\|\varphi\|^2\right) \tag{4.61}$$

for all $\varphi \in H^2(\mathbb{R}^d)$ and $t \in [0,T]$, where we choose ε', in accordance with the infinitesimal $-\Delta$-boundedness of $W_\infty(t)$, small enough such that (4.61) is well-defined.
Now we estimate the kinetic energy. As $\psi_t^\infty \in H^2(\mathbb{R}^d)$ for each t, we may insert ψ_t^∞ into (4.61) and obtain

$$\begin{aligned} \|\nabla\psi_t^\infty\|^2 = \langle\psi_t^\infty, -\Delta\psi_t^\infty\rangle &\leq (1-\varepsilon')^{-1}\left(|\langle U_\infty(t,t_0)\psi, H_\infty(t)U_\infty(t,t_0)\psi\rangle| + C'_\varepsilon\,\|\psi\|^2\right) \\ &= (1-\varepsilon')^{-1}\left(|\langle\psi, H_\infty(t)\psi\rangle| + C'_\varepsilon\,\|\psi\|^2\right), \end{aligned}$$

where we have used Lemma 4.7 and the unitarity of $U_\infty(t,t_0)$. Together with estimate (4.60), this finally yields

$$\|\nabla\psi_t^\infty\|^2 \leq \frac{1+\varepsilon'}{1-\varepsilon'}\,\|\nabla\psi\|^2 + \frac{2C'_\varepsilon}{1-\varepsilon'}\,\|\psi\|^2\,,$$

which proves (4.58)with

$$C = \max\left\{\frac{1+\varepsilon'}{1-\varepsilon'}, \frac{2C'_\varepsilon}{1-\varepsilon'}\right\}.$$

For (4.59) we proceed very similarly. Due to the infinitesimal $-\Delta$-boundedness of $W_\infty(t)$, we have for each $\varphi \in H^2(\mathbb{R}^d)$ and $t \in [0,T]$

$$\|H_\infty(t)\varphi\| \leq (1+\widetilde{\varepsilon})\,\|-\Delta\varphi\| + \widetilde{C_\varepsilon}\,\|\varphi\|\,. \tag{4.62}$$

On the other hand, we know from (4.30) that

$$\|-\Delta\varphi\| \leq \frac{\widetilde{C_\varepsilon}}{1-\widetilde{\varepsilon}}\,\|\varphi\| + \frac{1}{1-\widetilde{\varepsilon}}\,\|H_\infty(t)\varphi\| \tag{4.63}$$

for each $\varphi \in H^2(\mathbb{R}^d)$, $t \in [0,T]$. Analogously to above, we insert ψ_t^∞ into (4.63), implying

$$\begin{aligned}
\|-\Delta\psi_t^\infty\| &\leq \frac{\widetilde{C\varepsilon}}{1-\widetilde{\varepsilon}}\,\|\psi\| + \frac{1}{1-\widetilde{\varepsilon}}\,\|H_\infty(t)\psi\| \\
&\leq \frac{2\widetilde{C_\varepsilon}}{1-\widetilde{\varepsilon}}\,\|\psi\| + \frac{1+\widetilde{\varepsilon}}{1-\widetilde{\varepsilon}}\,\|-\Delta\psi\|
\end{aligned}$$

as a consequence of Lemma 4.7 and (4.62). The constant $\widetilde{C}$ in (4.59) is thus given as

$$\widetilde{C} = \max\left\{\frac{1+\widetilde{\varepsilon}}{1-\widetilde{\varepsilon}}, \frac{2\widetilde{C_\varepsilon}}{1-\widetilde{\varepsilon}}\right\}. \tag{4.64}$$

□

Lemma 4.8 provides us thus with a uniform bound on both $\|\nabla\psi_t^\infty\|$ and $\|-\Delta\psi_t^\infty\|$. Defining the constant

$$C_4 := \max\{C^{\frac{1}{2}}, \widetilde{C}\}, \tag{4.65}$$

we conclude

$$\begin{aligned}
\|\nabla\psi_t^\infty\| &\leq C_4\left(\|\psi\| + \|\nabla\psi\|\right), && (4.66)\\
\|-\Delta\psi_t^\infty\| &\leq C_4\left(\|\psi\| + \|-\Delta\psi\|\right). && (4.67)
\end{aligned}$$

This improves the bound from the last section as it is uniform in time. We could naturally achieve a uniform bound from Lemma 4.6 as well, by estimating $|t-t_0| \leq T$. This is however weaker than the statement of Lemma 4.8 as it comprises the quantity T, which is of no physical relevance and may be chosen arbitrarily large.

4.5 Proof of Part 2

We finally approach the last part of the proof: the strong convergence of the approximated towards the exact time evolution operator in the limit of large wavelengths. This part of the proof is taken from [12, 13], with the exception that we use our estimate of the kinetic energy $\|\nabla\psi_t^\infty\|^2$.

Consider first $\psi \in H^2(\mathbb{R}^d)$. We express the difference between the time evolution operators by the difference between their respective generators as

$$\begin{aligned}\big(U_\lambda(t,t_0) - U_\infty(t,t_0)\big)\psi &= -\int_{t_0}^{t} \partial_s\big(U_\lambda(t,s)U_\infty(s,t_0)\big)\psi\,ds \\ &= -i\int_{t_0}^{t} U_\lambda(t,s)\big(H_\lambda(s) - H_\infty(s)\big)U_\infty(s,t_0)\psi\,ds \\ &= \tfrac{2}{\omega}\int_{t_0}^{t} U_\lambda(t,s)\left(\mathbf{a}\left(\tfrac{\mathbf{x}}{\lambda},\omega s\right) - \mathbf{a}\left(0,\omega s\right)\right)\cdot\nabla U_\infty(s,t_0)\psi\,ds \\ &\quad - \tfrac{i}{\omega^2}\int_{t_0}^{t} U_\lambda(t,s)\left(\mathbf{a}\left(\tfrac{\mathbf{x}}{\lambda},\omega s\right)^2 - \mathbf{a}\left(0,\omega t\right)^2\right)U_\infty(s,t_0)\psi\,ds,\end{aligned}$$

where we have used part (d) of Theorem 3.38 for the derivative of $U_\lambda(t,s)$ and part (g) of Theorem 3.41 for the derivative of $U_\infty(s,t_0)$. As in the preceding section, we apply abbreviation (4.57), i.e. ψ_t^∞ is the wave function evolving from the initial state ψ under the time evolution generated by the Hamiltonian in dipole approximation.

Using the unitarity of $U_\lambda(t,s)$, we obtain

$$\begin{aligned}\left\|\big(U_\lambda(t,t_0) - U_\infty(t,t_0)\big)\psi\right\| &\le \tfrac{2}{\omega}\int_{t_0}^{t} \left\|\left(\mathbf{a}\left(\tfrac{\cdot}{\lambda},\omega s\right) - \mathbf{a}\left(0,\omega s\right)\right)\cdot\nabla\psi_s^\infty\right\| ds && (4.68)\\ &\quad + \tfrac{1}{\omega^2}\int_{t_0}^{t} \left\|\left(\mathbf{a}\left(\tfrac{\cdot}{\lambda},\omega s\right)^2 - \mathbf{a}\left(0,\omega s\right)^2\right)\psi_s^\infty\right\| ds. && (4.69)\end{aligned}$$

Clearly, $\mathbf{a}\left(\frac{\mathbf{x}}{\lambda},\omega s\right) - \mathbf{a}\left(0,\omega s\right) \to 0$ pointwise as $\lambda \to \infty$ with ω kept constant, hence part 2 of Theorem 4.1 follows immediately for $\psi \in H^2(\mathbb{R}^d)$ – if we can show that the theorem of dominated convergence applies to both (4.68) and (4.69). This is established in the ensuing claims.

Claim 1. *The theorem of dominated convergence applies to (4.68).*

Claim 2. *The theorem of dominated convergence applies to (4.69).*

Proof of Claim 2. The integral in (4.69) can be written as

$$\int_{t_0}^{t} ds \left(\int_{\mathbb{R}^d} d\mathbf{x} \left| \left(\mathbf{a}\left(\tfrac{\mathbf{x}}{\lambda}, \omega s\right)^2 - \mathbf{a}\left(0, \omega s\right)^2 \right) \psi_s^\infty(\mathbf{x}) \right|^2 \right)^{\frac{1}{2}} .$$

We show the applicability of the theorem of dominated convergence for the ds- and the $d\mathbf{x}$-integral separately.

Using the unitarity of $U_\infty(s,t_0)$, we estimate the integrand of the ds-integral as

$$\left\| \left(\mathbf{a}\left(\tfrac{\cdot}{\lambda}, \omega s\right)^2 - \mathbf{a}\left(0, \omega s\right)^2 \right) \psi_s^\infty \right\| \leq \left\| \mathbf{a}\left(\tfrac{\cdot}{\lambda}, \omega s\right)^2 - \mathbf{a}\left(0, \omega s\right)^2 \right\|_\infty \|\psi\| \leq 2C_{\mathbf{a}}^2 \|\psi\| ,$$

where the last step follows from assumption (A4). Thus we have identified a dominating function, which is obviously integrable over $s \in [t_0, t]$.

Analogously, the integrand of the $d\mathbf{x}$-integral is dominated by $2C_{\mathbf{a}}^2 |\psi_s(\mathbf{x})|^2$, which is integrable as

$$2C_{\mathbf{a}}^2 \int_{\mathbb{R}^d} d\mathbf{x}\, |\psi_s^\infty(\mathbf{x})|^2 = 2C_{\mathbf{a}}^2 \|\psi\|^2 < \infty.$$

□

Proof of Claim 1. Similarly to the proof of Claim 2, we show the existence of a dominating function first for the ds- and subsequently for the $d\mathbf{x}$-integral. Applying assumption (A4) and Lemma 4.8, we estimate the integrand of the ds-integral in (4.68) by

$$\begin{aligned} \left\| \left(\mathbf{a}\left(\tfrac{\cdot}{\lambda}, \omega s\right) - \mathbf{a}\left(0, \omega s\right) \right) \cdot \nabla \psi_s^\infty \right\| &\leq 2C_{\mathbf{a}} \|\nabla \psi_s^\infty\| \\ &\leq 2C_{\mathbf{a}} C_4 \left(\|\psi\| + \|\nabla \psi\| \right) , \end{aligned}$$

which is integrable over $[t_0, t]$ as $\psi \in H^2(\mathbb{R}^d)$. The integrand of the $d\mathbf{x}$-integral can be estimated in the same way. □

The only remaining step is now to generalise the result to $\psi \in L^2(\mathbb{R}^d)$. Let $\psi \in L^2(\mathbb{R}^d)$. Due to the density of $H^2(\mathbb{R}^d)$ in $L^2(\mathbb{R}^d)$ (Theorem 3.22), there is a sequence $\{\psi_k\}_{k\in\mathbb{N}} \subset H^2(\mathbb{R}^d)$ such that $\|\psi - \psi_k\| \leq \frac{1}{2k}$ for all $k \in \mathbb{N}$. Hence

$$\begin{aligned} &\left\| \left(U_\lambda(t,t_0) - U_\infty(t,t_0) \right) \psi \right\| \\ &\qquad \leq \left\| \left(U_\lambda(t,t_0) - U_\infty(t,t_0) \right) (\psi - \psi_k) \right\| + \left\| \left(U_\lambda(t,t_0) - U_\infty(t,t_0) \right) \psi_k \right\| \\ &\qquad \leq 2 \|\psi - \psi_k\| + \left\| \left(U_\lambda(t,t_0) - U_\infty(t,t_0) \right) \psi_k \right\| \\ &\qquad \leq \tfrac{1}{k} + \left\| \left(U_\lambda(t,t_0) - U_\infty(t,t_0) \right) \psi_k \right\| . \end{aligned} \tag{4.70}$$

The second term in (4.70) vanishes as $\lambda \to \infty$ because $\psi_k \in H^2(\mathbb{R}^d)$. Thus

$$\lim_{\substack{\lambda \to \infty \\ c \to \infty \\ \omega = const.}} \left\| \left(U_\lambda(t,t_0) - U_\infty(t,t_0) \right) \psi \right\| \leq \tfrac{1}{k}$$

for every $k \in \mathbb{N}$. This finally proves assertion (2) and concludes the proof of Theorem 4.1. □

5 Invariant Domains of the Hamiltonian in Dipole Approximation

Whereas we are able – in theory – to prepare the initial wave function in any (physical) state possible, it is a priori unclear how it will behave after some period of evolution under the Hamiltonian. Naturally this is very unsatisfying, and we will in this chapter put forth an effort to work out some properties of ψ_t. In groundwork for Chapter 6, we are especially interested in the decay of the wave function and its spatial derivatives.

Our approach to the problem will be in terms of invariant domains of the time evolution operator: in the knowledge that $H^2(\mathbb{R}^d)$ itself is left invariant by $U(t,s)$, we aim at recognising subspaces of $H^2(\mathbb{R}^d)$ with the same invariance property. Having just established the strong convergence of the exact towards the approximated time evolution, we content ourselves to examine the effects on ψ caused by the time evolution in dipole approximation.

The literature provides several works studying invariant subspaces for different choices of the Hamiltonian. In the time-independent case, Hunziker [48] deals with bounded smooth potentials, Radin and Simon [17] relax the conditions on V to relative (form-)boundedness, and Ozawa [49] identifies invariant subspaces related to weighted Sobolev spaces.
Explicitly time-dependent Hamiltonians are studied by Yajima [50], who in particular focuses on existence and regularity of the solutions of the Schrödinger equation, and Ozawa [51], who addresses the Hamiltonian of the AC-Stark Effect. Kuroda and Morita [52] examine exclusively bounded potentials, and Huang [18] identifies the (form-)domains of certain self-adjoint operators and their powers as invariant under the time evolution.
None of these results can immediately be applied to our case as $H_\infty(t)$ depends explicitly on time. What is more, also some of the conditions on the Hamiltonian are not met unless one restricts (A1) to smooth bounded potentials, or in the trivial case when the electromagnetic field equals zero.

Presumably the best one could hope for would be an invariance of the Schwartz space $\mathcal{S}(\mathbb{R}^d)$. This subset of $H^2(\mathbb{R}^d)$ is distinguished because all its elements are differentiable and display an ideal decay behaviour: they as well as all their partial derivatives decay faster than any inverse polynomial as $|\mathbf{x}| \to \infty$. However, this space is in general not left invariant by $U_\infty(t,t_0)$. The crucial point where the invariance fails is the potential $V(\mathbf{x})$ – assumption (A1) admits a very broad class of potentials, including such with L^2-integrable singularities, whose most relevant representative is the Coulomb potential.
To show that $\mathcal{S}(\mathbb{R}^d)$ is not left invariant, Radin and Simon [17] construct an element ψ of $\mathcal{S}(\mathbb{R}^d)$ for which $\langle \psi_t, |\mathbf{p}|^5 \psi_t \rangle$ becomes infinitely large in finite time, due to the local singularity of the Coulomb potential at $\mathbf{x} = 0$. Hence ψ_t does not possess the Schwartz property after some finite time t, although the original wave function ψ was an element of $\mathcal{S}(\mathbb{R}^d)$.

5.1 Invariance of the $\mathcal{C}^\infty$-functions for $H_\infty(t)$

Recalling the commutativity of $H_\infty(t)$ with the time evolution $U_\infty(s,t_0)$ established in Lemma 4.7, we are able to identify an invariant subspace of $H^2(\mathbb{R}^d)$ under the time evolution in dipole approximation: the **space of $\mathcal{C}^\infty$-functions of** $H(t)$,

$$\mathcal{C}^\infty\big(H(t)\big) := \bigcap_{n=1}^{\infty} \mathcal{D}\left(H(t)^n\right).$$

The following theorem establishes the invariance of this set.

Theorem 5.1. *Let $H_\infty(t)$ be the Hamiltonian in dipole approximation as in Theorem 4.1 and let $U_\infty(t,t_0)$ denote the time evolution operator generated by $H_\infty(t)$. Then*

$$U_\infty(t,t_0)\,\mathcal{C}^\infty\big(H_\infty(s)\big) = \mathcal{C}^\infty\big(H_\infty(s)\big),$$

and furthermore

$$\mathcal{C}^\infty\big(H_\infty(t_1)\big) = \mathcal{C}^\infty\big(H_\infty(t_2)\big)$$

for all $t_0, t, t_1, t_2, s \in [0,T]$, $t_0 \le t$.

Proof. For any $\psi \in \mathcal{D}(H_\infty(t)^n)$, Lemma 4.7 yields

$$\|H_\infty(t)^n U_\infty(s,t_0)\psi\| = \|U_\infty(s,t_0)H_\infty(t)^n\psi\| = \|H_\infty(t)^n\psi\| < \infty.$$

Thus $\mathcal{D}(H_\infty(t)^n)$ remains invariant under $U_\infty(s,t_0)$ for each n, which proves the first part of the theorem.
For the second part, we prove the hypothesis

$$\mathcal{D}\left(H_\infty(t_1)^n\right) = \mathcal{D}\left(H_\infty(t_2)^n\right) \tag{5.1}$$

for all $n \in \mathbb{N}$ via induction on n. The case $n = 1$ is clear. Now assume (5.1) holds for some $n > 1$. Then $\psi \in \mathcal{D}\left(H_\infty(t_1)^{n+1}\right)$ implies that $H_\infty(t_1)^n\psi \in \mathcal{D}(H_\infty(t_1)) = \mathcal{D}(H_\infty(t_2))$, and as the Hamiltonians commute, $H_\infty(t_2)\psi \in \mathcal{D}\left(H_\infty(t_1)^n\right) = \mathcal{D}\left(H_\infty(t_2)^n\right)$. Thus we conclude that $\psi \in \mathcal{D}\left(H_\infty(t_2)^{n+1}\right)$, which completes the induction. The second part of Theorem 5.1 is an immediate consequence of this. □

5.2 Invariance of the Domain of the Quantum Harmonic Oscillator

We now reveal the invariant subspace which is most relevant for Chapter 6, the domain of the quantum harmonic oscillator

$$\mathcal{D}\left(\mathbf{x}^2 + \mathbf{p}^2\right) = \left\{\psi \in L^2(\mathbb{R}^d) : (\mathbf{x}^2 + \mathbf{p}^2)\psi \in L^2(\mathbb{R}^d)\right\}.$$

The Hamiltonian $H_{\text{osc}} = \mathbf{x}^2 + \mathbf{p}^2$ is self-adjoint on this domain. A rigorous proof can be found in [53, Ch. 1.8] and [54, Ch. 5.14.5].
The general idea (for simplicity for dimension $d = 1$) is the following: one observes that the space

$$\widetilde{\mathcal{D}} := \{p(x)e^{-\frac{x^2}{2}} : p(x) \text{ polynomial}\} \subseteq \mathcal{D}\left(\mathbf{x}^2 + \mathbf{p}^2\right)$$

is not only dense in $L^2(\mathbb{R})$ but also invariant under H_{osc}. It is furthermore easy to see that H_{osc} is a symmetric operator on $\widetilde{\mathcal{D}}$. With creation and annihilation operator, one derives the normalised eigenfunctions of H_{osc},

$$\psi_n(x) = \frac{1}{2\sqrt{2^n n! \sqrt{\pi}}} H_n(x) e^{-\frac{\mathbf{x}^2}{2}} \tag{5.2}$$

as solutions of the equation

$$H_{\text{osc}}\, \psi_n(x) = \left(n + \frac{1}{2}\right) \psi_n(x).$$

$H_n(x)$ are the Hermite polynomials, given by

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}.$$

The normalised eigenfunctions $\{\psi_n\}_{n \in \mathbb{N}}$ form an orthonormal basis in $L^2(\mathbb{R})$ in which H_{osc} reduces to diagonal form. Hence we conclude that it is self-adjoint on the domain

$$\mathcal{D}(H_{\text{osc}}) = \left\{ \psi \in L^2(\mathbb{R}) : \sum_{n=0}^{\infty} \left| (n + \tfrac{1}{2}) \langle \psi, \psi_n \rangle \right|^2 < \infty \right\}.$$

Recalling the orthonormality of the eigenfunctions and the symmetry of H_{osc}, we can express this equivalently as

$$\sum_{n=0}^{\infty} \left| (n + \tfrac{1}{2}) \langle \psi, \psi_n \rangle \right|^2 = \left\| (\mathbf{x}^2 + \mathbf{p}^2)\psi \right\|^2.$$

In other words, $\left(\mathbf{x}^2 + \mathbf{p}^2, \mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)\right)$ is a self-adjoint extension of $\left(H_{\text{osc}}, \widetilde{\mathcal{D}}\right)$. The argument generalises easily to higher dimensions.

Before addressing the invariance of $\mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$, we state and show a lemma which is crucial for the proof.

Lemma 5.2.

$$\mathcal{D}\left(\mathbf{x}^2 + \mathbf{p}^2\right) = \mathcal{D}(\mathbf{x}^2) \cap \mathcal{D}(\mathbf{p}^2) \tag{5.3}$$

and

$$\left\|\mathbf{p}^2\varphi\right\|^2 + \left\|\mathbf{x}^2\varphi\right\|^2 \leq \left\|(\mathbf{x}^2 + \mathbf{p}^2)\varphi\right\|^2 + 2d\left\|\varphi\right\|^2 \tag{5.4}$$

for all $\varphi \in \mathcal{D}\left(\mathbf{x}^2 + \mathbf{p}^2\right)$.

In particular,

$$\begin{aligned}
&(a) & \left\|\mathbf{p}^2\varphi\right\|^2 &\leq \left\|(\mathbf{x}^2 + \mathbf{p}^2)\varphi\right\|^2 + 2d\left\|\varphi\right\|^2, \\
&(b) & \left\|\mathbf{x}^2\varphi\right\|^2 &\leq \left\|(\mathbf{x}^2 + \mathbf{p}^2)\varphi\right\|^2 + 2d\left\|\varphi\right\|^2, \\
&(c) & \left\|\mathbf{x}\cdot\mathbf{p}\varphi\right\|^2 &= \left\|\mathbf{p}\cdot\mathbf{x}\varphi\right\|^2 \\
&&&\leq \left\|\mathbf{x}^2\varphi\right\| \left\|\mathbf{p}^2\varphi\right\| + 2\left\||\mathbf{p}|\varphi\right\| \left\||\mathbf{x}|\varphi\right\| \\
&&&\leq (3d+2)\left(\left\|(\mathbf{x}^2 + \mathbf{p}^2)\varphi\right\|^2 + \left\|\varphi\right\|^2 \right).
\end{aligned}$$

The idea of the proof is the following: we note first that

$$\mathcal{D}\left(\mathbf{x}^2+\mathbf{p}^2\right) \supseteq \mathcal{D}\left(\mathbf{x}^2\right) \cap \mathcal{D}\left(\mathbf{p}^2\right)$$

as an immediate consequence of the triangle inequality. Then we show that $\|\mathbf{x}\cdot\mathbf{p}\varphi\|$ and $\|\mathbf{p}\cdot\mathbf{x}\varphi\|$ exist for any $\varphi \in \mathcal{D}\left(\mathbf{x}^2\right) \cap \mathcal{D}\left(\mathbf{p}^2\right)$. Using the thus gained knowledge that in this case $\mathbf{p}\varphi \in \mathcal{D}(\mathbf{x})$ and $\mathbf{x}\varphi \in \mathcal{D}(\mathbf{p})$, we arrive at an estimate yielding (5.4) – but only for $\varphi \in \mathcal{D}\left(\mathbf{x}^2\right) \cap \mathcal{D}\left(\mathbf{p}^2\right)$ –, therein relying on the commutation relation

$$[x_j, p_k] = i\delta_{jk}. \tag{5.5}$$

The inclusion $\subseteq$ in (5.3) is then implied by (5.4), which finally enables us to derive assertions (a) to (c).

Proof. Let $\varphi \in \mathcal{D}\left(\mathbf{x}^2\right) \cap \mathcal{D}\left(\mathbf{p}^2\right)$. Then

$$\left\|\left(\mathbf{x}^2+\mathbf{p}^2\right)\varphi\right\| \leq \left\|\mathbf{x}^2\varphi\right\| + \left\|\mathbf{p}^2\varphi\right\| < \infty,$$

hence

$$\mathcal{D}\left(\mathbf{x}^2+\mathbf{p}^2\right) \supseteq \mathcal{D}\left(\mathbf{x}^2\right) \cap \mathcal{D}\left(\mathbf{p}^2\right). \tag{5.6}$$

For $\varphi \in \mathcal{D}\left(\mathbf{x}^2\right) \cap \mathcal{D}\left(\mathbf{p}^2\right)$, it is a priori not clear whether $\mathbf{x}\cdot\mathbf{p}\varphi$ and $\mathbf{p}\cdot\mathbf{x}\varphi$ are elements of $L^2(\mathbb{R}^d)$, and consequently it is questionable whether the expressions $\|\mathbf{x}\cdot\mathbf{p}\varphi\|$ and $\|\mathbf{p}\cdot\mathbf{x}\varphi\|$ exist. Hence our first task is to provide proof that these objects are indeed well-defined; in other words, we need to show that $\mathbf{p}\varphi \in \mathcal{D}(\mathbf{x})$ and $\mathbf{x}\varphi \in \mathcal{D}(\mathbf{p})$.
Applying the Cauchy-Schwarz inequality in the Euclidean scalar product, we compute

$$\int\limits_{\mathbb{R}^d} |\mathbf{x}\cdot\mathbf{p}\varphi(\mathbf{x})|^2\, d\mathbf{x} \leq \int\limits_{\mathbb{R}^d} \mathbf{x}^2\, |\nabla\varphi(\mathbf{x})|^2\, d\mathbf{x} = \sum_{j=1}^{d} \int\limits_{\mathbb{R}^d} \mathbf{x}^2 \overline{\partial_j\varphi(\mathbf{x})}\partial_j\varphi(\mathbf{x}) d\mathbf{x}. \tag{5.7}$$

Formally, this can be expressed as

$$\sum_{j=1}^{d} \left\langle p_j\varphi, \mathbf{x}^2 p_j\varphi\right\rangle = \left\langle \mathbf{p}^2\varphi, \mathbf{x}^2\varphi\right\rangle + 2i\sum_{j=1}^{d} \left\langle p_j\varphi, x_j\varphi\right\rangle, \tag{5.8}$$

where we have used the commutation relation

$$[p_j, \mathbf{x}^2] = -2ix_j. \tag{5.9}$$

The existence of $\|\mathbf{x}\cdot\mathbf{p}\varphi\|$ is then easily established by means of the Cauchy-Schwarz inequality.
Caution should however be exercised when moving (self-adjoint) operators from one slot of an $L^2(\mathbb{R}^d)$-scalar product to the other. Whereas the right hand side of (5.7) is well-defined, (5.8) is not because $\mathbf{x}^2 p_j\varphi$ is not necessarily an element of $L^2(\mathbb{R}^d)$. In order to render (5.8) rigorous, we define the function

$$F_\varepsilon(\mathbf{x}) = \frac{\mathbf{x}^2}{1+\varepsilon\mathbf{x}^2}$$

and denote the corresponding multiplication operator by F_ε. The use of this operator is inspired by a work of Radin and Simon [17]. We claim that F_ε is a symmetric and bounded operator from $H^1(\mathbb{R}^d)$ to $H^1(\mathbb{R}^d)$, and prove this in Lemma 5.3 below. We then proceed as follows: observing that

$$F_\varepsilon(\mathbf{x}) \xrightarrow{\varepsilon\to 0} \mathbf{x}^2,$$

we show that the expression

$$\int_{\mathbb{R}^d} F_\varepsilon(\mathbf{x})\, |\nabla\varphi(\mathbf{x})|^2 \, d\mathbf{x} \tag{5.10}$$

is uniformly bounded in ε, hence the theorem of dominated convergence applies and we may consequently interchange the limit $\varepsilon \to 0$ and the integral. Thus it suffices to estimate (5.10), which we can handle in the spirit of (5.8) as F_ε maps into $H^1(\mathbb{R}^d)$.
Let us first establish the uniform boundedness of (5.10). We have

$$\begin{aligned}
(5.10) &= \sum_{j=1}^{d} \int_{\mathbb{R}^d} F_\varepsilon(\mathbf{x})\overline{\partial_j\varphi(\mathbf{x})}\partial_j\varphi(\mathbf{x})d\mathbf{x} \\
&= \sum_{j=1}^{d} \langle p_j\varphi, F_\varepsilon p_j\varphi\rangle \\
&= \sum_{j=1}^{d} \Big(\langle p_j^2\varphi, F_\varepsilon\varphi\rangle + \langle p_j\varphi, [F_\varepsilon, p_j]\,\varphi\rangle \Big),
\end{aligned}$$

where all terms are well-defined because, as a consequence of $\varphi \in \mathcal{D}(\mathbf{p}^2)$, we know that $F_\varepsilon\varphi \in H^1(\mathbb{R}^d)$, $F_\varepsilon p_j\varphi \in H^1(\mathbb{R}^d)$ and $p_jF_\varepsilon\varphi \in L^2(\mathbb{R}^d)$. The commutator

$$[F_\varepsilon, p_j] = i\partial_j F_\varepsilon = \frac{2ix_j}{(1+\varepsilon\mathbf{x}^2)^2} \tag{5.11}$$

is antisymmetric and bounded from $H^1(\mathbb{R}^d)$ to $H^1(\mathbb{R}^d)$ as a consequence of Lemma 5.3 below. Thus

$$\begin{aligned}
(5.10) &= \langle \mathbf{p}^2\varphi, F_\varepsilon\varphi\rangle + i\,\langle (\nabla F_\varepsilon)\cdot\mathbf{p}\varphi, \varphi\rangle \\
&= \left\langle \mathbf{p}^2\varphi, \frac{\mathbf{x}^2}{1+\varepsilon\mathbf{x}^2}\varphi\right\rangle + 2i\left\langle \frac{\mathbf{x}\cdot\mathbf{p}}{(1+\varepsilon\mathbf{x}^2)^2}\varphi, \varphi\right\rangle \\
&\le \langle \mathbf{p}^2\varphi, \mathbf{x}^2\varphi\rangle + 2\left|\left\langle |\mathbf{p}|\varphi, \frac{|\mathbf{x}|}{(1+\varepsilon\mathbf{x}^2)^2}\varphi\right\rangle\right|.
\end{aligned} \tag{5.12}$$

This can be upper bounded by

$$(5.10) \le \left\|\mathbf{p}^2\varphi\right\| \left\|\mathbf{x}^2\varphi\right\| + 2\,\||\mathbf{p}|\varphi\|\,\||\mathbf{x}|\varphi\| < \infty, \tag{5.13}$$

where we have used the estimates

$$\frac{\mathbf{x}^2}{1+\varepsilon\mathbf{x}^2} \le \mathbf{x}^2 \quad \text{and} \quad \frac{|\mathbf{x}|}{(1+\varepsilon\mathbf{x}^2)^2} \le |\mathbf{x}| \quad \forall\, \mathbf{x}\in\mathbb{R}^d. \tag{5.14}$$

Clearly, (5.13) is bounded uniformly in ε, hence the theorem of dominated convergence applies in (5.10). We thus obtain for (5.7)

$$\begin{aligned}\int_{\mathbb{R}^d} |\mathbf{x}\cdot\mathbf{p}\varphi(\mathbf{x})|^2\,d\mathbf{x} &\leq \lim_{\varepsilon\to 0}\int_{\mathbb{R}^d} F_\varepsilon(\mathbf{x})\,|\nabla\varphi(\mathbf{x})|^2\,d\mathbf{x} \\ &\leq \left\|\mathbf{p}^2\varphi\right\|\left\|\mathbf{x}^2\varphi\right\| + 2\,\||\mathbf{p}|\varphi\|\,\||\mathbf{x}|\varphi\|\,,\end{aligned} \tag{5.15}$$

hence $\|\mathbf{x}\cdot\mathbf{p}\varphi\|$ exists for any $\varphi\in\mathcal{D}\left(\mathbf{x}^2\right)\cap\mathcal{D}\left(\mathbf{p}^2\right)$.
From this result we conclude that $\|\mathbf{p}\cdot\mathbf{x}\varphi\|$ is also well-defined, as

$$\begin{aligned}\int_{\mathbb{R}^d} |\mathbf{p}\cdot\mathbf{x}\varphi(\mathbf{x})|^2 d\mathbf{x} &= \int_{\mathbb{R}^d} |\mathbf{x}\cdot\mathbf{p}\varphi(\mathbf{x}) - id\varphi(\mathbf{x})|^2 d\mathbf{x} \\ &\leq \left(\|\mathbf{x}\cdot\mathbf{p}\varphi\| + d\,\|\varphi\|\right)^2 < \infty,\end{aligned}$$

hence

$$\begin{aligned}\|\mathbf{p}\cdot\mathbf{x}\varphi\|^2 &= \langle\mathbf{x}\cdot\mathbf{p}\varphi - id\varphi, \mathbf{x}\cdot\mathbf{p}\varphi - id\varphi\rangle \\ &= \|\mathbf{x}\cdot\mathbf{p}\varphi\|^2 + d^2\,\|\varphi\|^2 + id\,\langle\varphi,[\mathbf{x},\mathbf{p}]\varphi\rangle \\ &= \|\mathbf{x}\cdot\mathbf{p}\varphi\|^2\,.\end{aligned} \tag{5.16}$$

With (5.15) and (5.16), we can now prove (5.4) for $\varphi\in\mathcal{D}\left(\mathbf{x}^2\right)\cap\mathcal{D}\left(\mathbf{p}^2\right)$. Consider

$$\left\|(\mathbf{x}^2+\mathbf{p}^2)\varphi\right\|^2 - \left\|\mathbf{p}^2\varphi\right\|^2 = \left\|\mathbf{x}^2\varphi\right\|^2 + \left\langle\mathbf{p}^2\varphi,\mathbf{x}^2\varphi\right\rangle + \left\langle\mathbf{x}^2\varphi,\mathbf{p}^2\varphi\right\rangle. \tag{5.17}$$

Let us first examine the third term in (5.17). **Formally**, one computes

$$\begin{aligned}\left\langle\mathbf{p}^2\varphi,\mathbf{x}^2\varphi\right\rangle &= \sum_{j=1}^{d}\left\langle\varphi,p_j^2\mathbf{x}^2\varphi\right\rangle = \sum_{j=1}^{d}\Big(\left\langle\varphi,p_j\mathbf{x}^2p_j\varphi\right\rangle + \left\langle\varphi,p_j[p_j,\mathbf{x}^2]\varphi\right\rangle\Big) \\ &= \sum_{j,k=1}^{d}\|x_kp_j\varphi\|^2 - 2i\sum_{j=1}^{d}\langle\varphi,p_jx_j\varphi\rangle\,,\end{aligned} \tag{5.18}$$

but has to deal with the same problems of ill-definedness as in (5.8). Hence we take again the detour via the bounded operator F_ε and compute with (5.11)

$$\begin{aligned}\left\langle\mathbf{p}^2\varphi,F_\varepsilon\varphi\right\rangle &= \sum_{j=1}^{d}\langle p_j\varphi,p_jF_\varepsilon\varphi\rangle \\ &= \sum_{j=1}^{d}\Big(\langle p_j\varphi,F_\varepsilon p_j\varphi\rangle + \langle p_j\varphi,[p_j,F_\varepsilon]\varphi\rangle \\ &= \sum_{j=1}^{d}\left(\langle p_j\varphi,F_\varepsilon p_j\varphi\rangle - 2i\left\langle p_j\varphi,\frac{x_j}{(1+\varepsilon\mathbf{x}^2)^2}\varphi\right\rangle\right).\end{aligned}$$

The expression is clearly bounded uniformly in ε as $\left|\left\langle\mathbf{p}^2\varphi,F_\varepsilon\varphi\right\rangle\right| \leq \left\|\mathbf{p}^2\varphi\right\|\left\|\mathbf{x}^2\varphi\right\|$. Hence

$$\begin{aligned}\left\langle\mathbf{p}^2\varphi,\mathbf{x}^2\varphi\right\rangle &= \lim_{\varepsilon\to 0}\left\langle\mathbf{p}^2\varphi,F_\varepsilon\varphi\right\rangle \\ &= \sum_{j,k=1}^{d}\|x_kp_j\varphi\|^2 - 2i\sum_{j=1}^{d}\langle\varphi,p_jx_j\varphi\rangle\,.\end{aligned} \tag{5.19}$$

Analogously, we obtain

$$\left\langle \mathbf{x}^2\varphi, \mathbf{p}^2\varphi \right\rangle = \sum_{j,k=1}^{d} \|x_k p_j \varphi\|^2 + 2i \sum_{j=1}^{d} \langle \varphi, x_j p_j \varphi \rangle . \tag{5.20}$$

Insertion of (5.19) and (5.20) into (5.17) yields

$$\begin{aligned} \left\|(\mathbf{x}^2 + \mathbf{p}^2)\varphi\right\|^2 &= \left\|\mathbf{p}^2\varphi\right\|^2 + \left\|\mathbf{x}^2\varphi\right\|^2 + 2 \sum_{j,k=1}^{d} \|x_k p_j \varphi\|^2 + 2i \sum_{j=1}^{d} \langle \varphi, [x_j, p_j]\varphi \rangle \\ &\geq \left\|\mathbf{p}^2\varphi\right\|^2 + \left\|\mathbf{x}^2\varphi\right\|^2 - 2d\,\|\varphi\|^2 , \end{aligned} \tag{5.21}$$

proving (5.4) for $\varphi \in \mathcal{D}\left(\mathbf{x}^2\right) \cap \mathcal{D}\left(\mathbf{p}^2\right)$.

With this result we can show (5.3): From (5.21) it is clear that $\varphi \in \mathcal{D}\left(\mathbf{x}^2 + \mathbf{p}^2\right)$ implies $\varphi \in \mathcal{D}\left(\mathbf{x}^2\right) \cap \mathcal{D}\left(\mathbf{p}^2\right)$, which together with (5.6) proves the statement. Naturally all estimates made so far are thus automatically valid for $\varphi \in \mathcal{D}\left(\mathbf{x}^2 + \mathbf{p}^2\right)$, yielding (5.4) without any restriction.

Assertions (a) and (b) are an immediate consequence of (5.4). In order to verify (c), we apply (a) and (b) to (5.15) and obtain

$$\begin{aligned} \|\mathbf{x}\cdot\mathbf{p}\varphi\|^2 = \|\mathbf{p}\cdot\mathbf{x}\varphi\|^2 &\leq \tfrac{1}{2}\left\|\mathbf{x}^2\varphi\right\|^2 + \tfrac{1}{2}\left\|\mathbf{p}^2\varphi\right\|^2 + \left\||\mathbf{x}^2|\varphi\right\|^2 + \left\||\mathbf{p}^2|\varphi\right\|^2 \\ &\leq \tfrac{3}{2}\left\|(\mathbf{x}^2 + \mathbf{p}^2)\varphi\right\|^2 + (3d+2)\,\|\varphi\|^2 \\ &\leq (3d+2)\left(\left\|(\mathbf{x}^2 + \mathbf{p}^2)\varphi\right\|^2 + \|\varphi\|^2\right), \end{aligned} \tag{5.22}$$

where we have used the estimate (4.19) and

$$\||\mathbf{x}|\varphi\|^2 \leq \left\|\mathbf{x}^2\varphi\right\|^2 + \|\varphi\|^2$$

and

$$\||\mathbf{p}|\varphi\|^2 \leq \left\|\mathbf{p}^2\varphi\right\|^2 + \|\varphi\|^2 .$$

□

We still need to prove the boundedness of F_ε and $\partial_j F_\varepsilon$. Naturally the bound will not be uniform in ε, as $F_\varepsilon \xrightarrow{\varepsilon\to 0} \mathbf{x}^2$ and $\mathbf{x}^2$ is unbounded on $H^1(\mathbb{R}^d)$.

Lemma 5.3. *Let $\varepsilon > 0$. Define*

$$\begin{aligned} F_\varepsilon : \mathbb{R}^d &\longrightarrow \mathbb{R} \\ \mathbf{x} &\longmapsto F_\varepsilon(\mathbf{x}) = \frac{\mathbf{x}^2}{1+\varepsilon\mathbf{x}^2} \end{aligned}$$

and let F_ε denote the corresponding multiplication operator. Analogously, $\partial_j F_\varepsilon$ is the multiplication operator corresponding to

$$\partial_j F_\varepsilon(\mathbf{x}) = \frac{2x_j}{(1+\varepsilon\mathbf{x}^2)^2}$$

for $j = 1, \dots, d$. Then the restrictions of F_ε and $\partial_j F_\varepsilon$ to $H^1(\mathbb{R}^d)$ are symmetric and bounded as operators from $H^1(\mathbb{R}^d)$ to $H^1(\mathbb{R}^d)$.

Proof. The symmetry of both F_ε and $\partial_j F_\varepsilon$ is obvious as they are multiplication operators corresponding to real-valued functions. To show the boundedness of F_ε, let $\psi \in H^1(\mathbb{R}^d)$. According to the definition of the Sobolev norm,

$$\|F_\varepsilon \psi\|^2 = \|F_\varepsilon \psi\|^2 + \|\nabla (F_\varepsilon \psi)\|^2 . \tag{5.23}$$

The first term in (5.23) can be estimated as

$$\|F_\varepsilon \psi\|^2 = \int\limits_{\mathbb{R}^d} \left| \frac{\mathbf{x}^2}{1+\varepsilon \mathbf{x}^2} \psi(\mathbf{x}) \right|^2 d\mathbf{x} \leq \frac{1}{\varepsilon^2} \|\psi\|^2 , \tag{5.24}$$

where we have used the approximation

$$\frac{\mathbf{x}^2}{1+\varepsilon \mathbf{x}^2} = \frac{1}{\varepsilon}\left(1 - \frac{1}{1+\varepsilon \mathbf{x}^2}\right) \leq \frac{1}{\varepsilon}. \tag{5.25}$$

With (5.25) and the fact that $(1+\varepsilon \mathbf{x}^2)^{-3} \leq 1$, we compute for the second term in (5.23)

$$\begin{aligned}
\|\nabla (F_\varepsilon \psi)\|^2 &= \sum_{j=1}^{d} \|(\partial_j F_\varepsilon)\psi + F_\varepsilon \partial_j \psi\|^2 \\
&\leq 2 \sum_{j=1}^{d} \left(\|(\partial_j F_\varepsilon)\psi\|^2 + \|F_\varepsilon \partial_j \psi\|^2 \right) \\
&= 2 \int\limits_{\mathbb{R}^d} \frac{4\mathbf{x}^2}{(1+\varepsilon \mathbf{x}^2)^4} |\psi(\mathbf{x})|^2 d\mathbf{x} + 2 \sum_{j=1}^{d} \int\limits_{\mathbb{R}^d} \frac{1}{\varepsilon^2} |\partial_j \psi(\mathbf{x})|^2 d\mathbf{x} \\
&\leq \frac{8}{\varepsilon} \|\psi\|^2 + \frac{2}{\varepsilon^2} \|\nabla \psi\|^2 ,
\end{aligned} \tag{5.26}$$

where we have in the second line used the estimate $(c+d)^2 \leq 2(c^2+d^2)$ for $c, d \geq 0$ as a consequence of (4.19). Together, (5.24) and (5.26) yield

$$\|F_\varepsilon\|^2_{H^1(\mathbb{R}^d) \to H^1(\mathbb{R}^d)} = \sup_{\substack{\psi \in H^1(\mathbb{R}^d) \\ \psi \neq 0}} \frac{\|F_\varepsilon \psi\|^2_{H^1(\mathbb{R}^d)}}{\|\psi\|^2_{H^1(\mathbb{R}^d)}} \leq C \left(\frac{1}{\varepsilon^2} + \frac{1}{\varepsilon} \right) ,$$

proving the boundedness of F_ε.
For $\partial_j F_\varepsilon$, we proceed analogously. Using the same reasoning as in (5.26), we compute

$$\begin{aligned}
\|(\partial_j F_\varepsilon)\psi\|^2_{H^1(\mathbb{R}^d)} &= \|(\partial_j F_\varepsilon)\psi\|^2 + \|\nabla ((\partial_j F_\varepsilon)\psi)\|^2 \\
&\leq \frac{C}{\varepsilon} \|\psi\|^2 + \sum_{k=1}^{d} \|(\partial_k \partial_j F_\varepsilon)\psi + (\partial_j F_\varepsilon)(\partial_k \psi)\|^2 \\
&\leq \frac{C}{\varepsilon} \|\psi\|^2 + 2 \sum_{k=1}^{d} \|(\partial_k \partial_j F_\varepsilon)\psi\|^2 + 2 \sum_{k=1}^{d} \|(\partial_j F_\varepsilon)(\partial_k \psi)\|^2 .
\end{aligned} \tag{5.27}$$

With

$$\partial_k \partial_j F_\varepsilon(\mathbf{x}) = \frac{2\delta_{kj}}{(1+\varepsilon \mathbf{x}^2)^2} - \frac{8\varepsilon x_k x_j}{(1+\varepsilon \mathbf{x}^2)^3},$$

the second term in (5.27) can be estimated as

$$\begin{aligned}
2\sum_{k=1}^{d} \|\partial_k \partial_j F_\varepsilon)\psi\|^2 &\leq 2\sum_{k=1}^{d} \int\limits_{\mathbb{R}^d} \left| 2\delta_{kj} - 8\varepsilon \frac{x_k x_j}{(1+\varepsilon \mathbf{x}^2)^2} \right|^2 |\psi(\mathbf{x})|^2 d\mathbf{x} \\
&\leq C \sum_{k=1}^{d} \int\limits_{\mathbb{R}^d} \left(\delta_{kj} + \varepsilon^2 \frac{x_k^2 x_j^2}{(1+\varepsilon \mathbf{x}^2)^2} + \delta_{kj} \varepsilon \frac{x_j^2}{1+\varepsilon \mathbf{x}^2} \right) |\psi(\mathbf{x})|^2 d\mathbf{x} \\
&\leq C \|\psi\|^2 .
\end{aligned}$$

For the third term in (5.27), we obtain

$$2\sum_{k=1}^{d} \|(\partial_j F_\varepsilon)(\partial_k \psi)\|^2 \leq \frac{C}{\varepsilon} \|\nabla\psi\|^2 .$$

Together, this yields

$$\|(\partial_j F_\varepsilon)\psi\|^2_{H^1(\mathbb{R}^d)} \leq C \left(\|\psi\|^2 + \frac{1}{\varepsilon} \|\nabla\psi\|^2 \right),$$

thus

$$\|\partial_j F_\varepsilon\|^2_{H^1(\mathbb{R}^d)\to H^1(\mathbb{R}^d)} \leq C \left(1 + \frac{1}{\varepsilon}\right),$$

which finally proves the lemma. □

Based on Lemma 5.2, we can now state and prove a theorem yielding the invariance of the domain $\mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$ of the quantum harmonic oscillator under the time evolution $U_\infty(t, t_0)$. This space is characterised by the span of the normalised eigenfunctions (5.2), which provides a core for $\mathbf{x}^2 + \mathbf{p}^2$. More important for our purposes is however the observation that the functions in $\mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$ have finite second and fourth momenta in both position and momentum, i.e.

$$\begin{aligned}
\langle \psi, \mathbf{x}^2 \psi \rangle &= \||\mathbf{x}|\psi\|^2 < \infty, \quad \langle \psi, \mathbf{x}^4 \psi \rangle = \left\|\mathbf{x}^2 \psi\right\|^2 < \infty, \\
\langle \psi, \mathbf{p}^2 \psi \rangle &= \|\nabla\psi\|^2 < \infty\,, \quad \langle \psi, \mathbf{p}^4 \psi \rangle = \|-\Delta\psi\|^2 < \infty
\end{aligned} \tag{5.28}$$

for each $\psi \in \mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$. The invariance of $\mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$ – which we will prove now – implies that the property (5.28) is maintained under the time evolution: starting with an initial wave function in $\mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$ we may be assured that none of the time-evolved moments (5.28) will ever diverge.

Theorem 5.4. *Let $H_\infty(t)$ and $U_\infty(t, t_0)$ be defined as in Theorem 4.1. Then*

$$U_\infty(t, t_0)\mathcal{D}\left(\mathbf{x}^2 + \mathbf{p}^2\right) = \mathcal{D}\left(\mathbf{x}^2 + \mathbf{p}^2\right), \tag{5.29}$$

i.e. $\mathcal{D}\left(\mathbf{x}^2 + \mathbf{p}^2\right)$ is invariant under $U_\infty(t, t_0)$.

The idea for the proof is taken from HUANG [18, Theorem 3.1], and has been adapted to the situation at hand. We apply the most general version of KATO's theorem (Theorem 3.41) to $X \equiv L^2(\mathbb{R}^d)$ and $A(t) \equiv iH_\infty(t)$, but this time do not choose Y as the domain of $H_\infty(t)$. Instead, we take the space $\mathcal{D}\left(\mathbf{x}^2 + \mathbf{p}^2\right)$, which is made a Banach space by endowing it with the graph norm of $\mathbf{x}^2 + \mathbf{p}^2$. The inclusion $\subseteq$ in (5.29) is then a consequence of assertion (e) of Theorem 3.41.

Proof of Theorem 5.4. Define the graph norm

$$\|\cdot\|_D := \|\cdot\| + \left\|(\mathbf{x}^2 + \mathbf{p}^2)\cdot\right\|. \tag{5.30}$$

As $\mathbf{x}^2 + \mathbf{p}^2$ is a self-adjoint operator, the space

$$D := \left(\mathcal{D}\left(\mathbf{x}^2 + \mathbf{p}^2\right), \|\cdot\|_{\mathcal{D}}\right)$$

is a Banach space according to Lemma 3.4. It is continuously embedded into $L^2(\mathbb{R}^d)$ as

$$\|\mathbb{1}\|_{D\to L^2(\mathbb{R}^d)} = \sup_{\substack{\psi\in D\\ \psi\neq 0}} \frac{\|\psi\|}{\|\psi\|_D} = \sup_{\substack{\psi\in D\\ \psi\neq 0}} \frac{\|\psi\|}{\|\psi\| + \|(\mathbf{x}^2 + \mathbf{p}^2)\psi\|} \leq 1. \tag{5.31}$$

D is dense in $L^2(\mathbb{R}^d)$ because $\mathcal{S}(\mathbb{R}^d) \subseteq D$ and $\mathcal{S}(\mathbb{R}^d)$ is dense in $L^2(\mathbb{R}^d)$. Thus the basic requirements of Theorem 3.41 are met.

Whereas assumption (i) of Theorem 3.38 has already been verified in the previous chapter, (iii) needs to be shown for D. The requirement $D \subseteq H^2(\mathbb{R}^d)$ is an immediate consequence of Lemma 5.2. In order to prove the rest of (iii), we need the following auxiliary lemma.

Lemma 5.5. *Let $W_\infty(t)$ be defined as in Chapter 4. Then*

$$W_\infty(t) << \mathbf{x}^2 + \mathbf{p}^2.$$

As a consequence, $H_\infty(t) + \mathbf{x}^2$ is self-adjoint on D.

Proof. We already know that $W_\infty(t) << \mathbf{p}^2$ (Lemma 4.4). Hence condition (i) of the definition of infinitesimal boundedness (Definition 3.6) is clearly fulfilled, as each element φ of $\mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$ is also in $\mathcal{D}(-\Delta)$. Thus there exist $0 < \varepsilon, C_\varepsilon < \infty$ such that

$$\|W_\infty(t)\varphi\| \leq \varepsilon \left\|\mathbf{p}^2\varphi\right\| + C_\varepsilon \|\varphi\| < \infty.$$

The second requirement of infinitesimal boundedness follows immediately from Lemma 5.2, as

$$\|W_\infty(t)\varphi\| \leq \varepsilon \left\|(\mathbf{x}^2 + \mathbf{p}^2)\varphi\right\| + (2d + C_\varepsilon) \|\varphi\|. \tag{5.32}$$

The last statement of Lemma 5.5 is a direct consequence of the KATO-RELLICH theorem (Theorem 3.8). □

Now we verify assumption (iii). We must show that $iH_\infty(t) \in \mathcal{L}(D, L^2(\mathbb{R}^d))$ and that $t \mapsto iH_\infty(t)$ is norm-continuous with respect to $\|\cdot\|_{D\to L^2(\mathbb{R}^d)}$. The former holds true since

$$\begin{aligned}
\|H_\infty(t)\|_{D\to L^2(\mathbb{R}^d)} &\le \sup_{\substack{\psi\in D\\ \psi\neq 0}} \frac{\left\|\mathbf{p}^2\psi\right\| + \|W_\infty(t)\psi\|}{\|\psi\|_D} \\
&\le \sup_{\substack{\psi\in D\\ \psi\neq 0}} \frac{(1+\varepsilon)\left\|(\mathbf{p}^2+\mathbf{x}^2)\psi\right\| + (4d + C_\varepsilon)\|\psi\|}{\|\psi\|_D} \\
&\le 4d + C_\varepsilon + \varepsilon,
\end{aligned}$$

where we have used (5.32) and Lemma 5.2a. With the abbreviation $\|\cdot\|_{D\to L^2(\mathbb{R}^d)} \equiv \|\cdot\|_{\mathrm{op}}$, we compute

$$\left\|\mathbf{p}^2\right\|_{\mathrm{op}} = \sup_{\substack{\psi\in D\\ \psi\neq 0}} \frac{\left\|\mathbf{p}^2\psi\right\|}{\|\psi\|_D} \le \sup_{\substack{\psi\in D\\ \psi\neq 0}} \frac{\left\|(\mathbf{p}^2+\mathbf{x}^2)\psi\right\| + 2d\,\|\psi\|}{\|\psi\|_D} \le 2d, \tag{5.33}$$

and consequently

$$\||\mathbf{p}|\|_{\mathrm{op}} \le \left\|\mathbb{1} + \mathbf{p}^2\right\|_{\mathrm{op}} \le 1 + 2d. \tag{5.34}$$

Hence

$$\begin{aligned}
\|H_\infty(t_1) - H_\infty(t_2)\|_{\mathrm{op}} &\le \tfrac{2}{\omega}|\mathbf{a}(0,\omega t_1) - \mathbf{a}(0,\omega t_2)|\,\||\mathbf{p}|\|_{\mathrm{op}} + \tfrac{1}{\omega^2}\left|\mathbf{a}(0,\omega t_1)^2 - \mathbf{a}(0,\omega t_2)^2\right|\|\mathbb{1}\|_{\mathrm{op}} \\
&\le \tfrac{2}{\omega}(1+2d)|\mathbf{a}(0,\omega t_1) - \mathbf{a}(0,\omega t_2)| + \tfrac{1}{\omega^2}\left|\mathbf{a}(0,\omega t_1)^2 - \mathbf{a}(0,\omega t_2)^2\right|,
\end{aligned}$$

which implies the norm continuity as a consequence of the mean value theorem, analogously to (4.36) to (4.39) in Chapter 4.2.3.

It remains to verify condition (ii”) of Theorem 3.41. To this end, we define

$$S(t) := i(H_\infty(t) + \mathbf{x}^2) + \mathbb{1}.$$

This is an isomorphism because, according to the Hille-Yosida theorem (Theorem 3.31), $1 \in \rho(-i(H_\infty(t) + \mathbf{x}^2))$ as $H_\infty(t) + \mathbf{x}^2$ is self-adjoint. The fact that $t \mapsto S(t)$ is continuously differentiable with respect to $\|\cdot\|_{\mathrm{op}}$ can be seen analogously to section 4.2.4, (4.42) to (4.44), using (5.31) and (5.34).
Our aim is it now to find an operator $B(t) \in \mathcal{L}(L^2(\mathbb{R}^d))$ such that $S(t)iH_\infty(t)S(t)^{-1} = iH_\infty(t) + B(t)$. We rewrite

$$S(t)iH_\infty(t)S(t)^{-1} = iH_\infty(t) + [S(t), iH_\infty(t)]\,S(t)^{-1}.$$

The commutator can be computed as

$$\left[i(H_\infty(t) + \mathbf{x}^2) + \mathbb{1}, iH_\infty(t)\right] = -\left[\mathbf{x}^2, H_\infty(t)\right] = \tfrac{4i}{\omega}\mathbf{a}\,(0,\omega t)\cdot\mathbf{x} - 2i\{\mathbf{x},\mathbf{p}\}.$$

Thus we obtain

$$B(t) = \left(\tfrac{4i}{\omega}\mathbf{a}\,(0,\omega t)\cdot\mathbf{x} - 2i\{\mathbf{x},\mathbf{p}\}\right)S(t)^{-1}.$$

Before we can show that $B(t)$ is indeed bounded, we need to prove a lemma which is analogue to Lemma 4.5, establishing the uniform equivalence of the graph norm of $H(t)$ and the Sobolev norm. Here, D plays the role of $H^2(\mathbb{R}^d)$ whereas $H_\infty(t) + \mathbf{x}^2$ corresponds to $H(t)$.

Lemma 5.6. *There exists a constant $C > 0$ such that $\|\cdot\|_D \leq C \|\cdot\|_{H_\infty(t)+\mathbf{x}^2}$ uniformly in t.*

Proof. Let $\psi \in D$ and let ε and C_ε denote the coefficients of infinitesimal $\mathbf{x}^2+\mathbf{p}^2$-boundedness of $W_\infty(t)$. Then

$$\left\|(H_\infty(t) + \mathbf{x}^2)\psi\right\| \geq \left\|(\mathbf{p}^2 + \mathbf{x}^2)\psi\right\| - \|W_\infty(t)\psi\| \geq (1 - \varepsilon) \left\|(\mathbf{p}^2 + \mathbf{x}^2)\psi\right\| - C_\varepsilon \|\psi\|,$$

hence

$$\left\|(\mathbf{p}^2 + \mathbf{x}^2)\psi\right\| + \|\psi\| \leq \frac{1}{1-\varepsilon} \left\|(H_\infty(t) + \mathbf{x}^2)\psi\right\| + \left(\frac{C_\varepsilon}{1-\varepsilon} + 1\right) \|\psi\|,$$

implying the statement of the lemma. □

The operator norm of $B(t)$ on $L^2(\mathbb{R}^d)$ is given by

$$\begin{aligned}\|B(t)\| &\leq \left(2 \|\{\mathbf{x}, \mathbf{p}\}\|_{D\to L^2(\mathbb{R}^d)} + \tfrac{4}{\omega} C_{\mathbf{a}} \||\mathbf{x}|\|_{D\to L^2(\mathbb{R}^d)}\right) \left\|S(t)^{-1}\right\|_{L^2(\mathbb{R}^d)\to D} \\ &\leq C \left\|S(t)^{-1}\right\|_{L^2(\mathbb{R}^d)\to D},\end{aligned} \tag{5.35}$$

with $C_{\mathbf{a}}$ as in (4.24). We have for this purpose exploited that

$$\|\{\mathbf{x}, \mathbf{p}\}\|_{D\to L^2(\mathbb{R}^d)} \leq 2 \|\mathbf{x} \cdot \mathbf{p}\|_{D\to L^2(\mathbb{R}^d)} \leq 2\sqrt{3d+2} \tag{5.36}$$

due to Lemma 5.2, and that

$$\||\mathbf{x}|\|_{D\to L^2(\mathbb{R}^d)} \leq 1 + \left\|\mathbf{x}^2\right\|_{D\to L^2(\mathbb{R}^d)} \leq 2d + 1 \tag{5.37}$$

analogously to 5.34. In accordance with Lemma 5.6, the norm of $S(t)^{-1}$ can be estimated as

$$\begin{aligned}&\left\|S(t)^{-1}\right\|_{L^2(\mathbb{R}^d)\to D} \\ &\leq C \sup_{\substack{\psi\in L^2(\mathbb{R}^d)\\ \psi\neq 0}} \frac{\left\|i(H_\infty(t) + \mathbf{x}^2)\left[i(H_\infty(t) + \mathbf{x}^2) + \mathbb{1}\right]^{-1}\psi\right\| + \left\|R_1(-i(H_\infty(t) + \mathbf{x}^2)\right\|}{\|\psi\|} \\ &\leq 3C,\end{aligned}$$

analogously to the reasoning that led to (4.34). Inserting this result into (5.35), we conclude that $B(t)$ is bounded uniformly in t.

The last step is to verify that $t \mapsto B(t)$ is strongly continuous. From (5.35) we observe that for some constant C,

$$\|B(t_1) - B(t_2)\| \leq C \left\|S(t_1)^{-1} - S(t_2)^{-1}\right\|_{L^2(\mathbb{R}^d)\to D}, \tag{5.38}$$

thus it suffices to establish the strong continuity of $t \mapsto S(t)$. This is due to the second resolvent identity (Theorem 3.13), as

$$\begin{aligned}\left\|S(t_1)^{-1} - S(t_2)^{-1}\right\|_{L^2(\mathbb{R}^d)\to D} &= \left\|R_1(-i(H_\infty(t_1) + \mathbf{x}^2)) - R_1(-i(H_\infty(t_2) + \mathbf{x}^2))\right\|_{L^2(\mathbb{R}^d)\to D} \\ &= \left\|S(t_1)^{-1}(H_\infty(t_1) - H_\infty(t_2))S(t_2)^{-1}\right\|_{L^2(\mathbb{R}^d)\to D} \\ &\leq C \|H_\infty(t_1) - H_\infty(t_2)\|_{D\to L^2(\mathbb{R}^d)}\end{aligned}$$

for some constant C, due to the uniform boundedness of $S(t)^{-1}$. The continuity of $t \mapsto B(t)\psi$ for any $\psi \in D$ is therefore implied by the norm-continuity of $t \mapsto H_\infty(t)$, which was established in Chapter 4.

It only remains to show the inclusion $\supseteq$ in (5.29), which is according to the semigroup property equivalent to the statement that

$$U_\infty(t_0, t)D \subseteq D.$$

One can perform the proof of KATO's theorem (Theorem 3.38) with the roles of t and s exchanged, and thus derive a unitary time evolution $U(t,s)^* = U(s,t)$ for $t \geq s$, which displays the same properties as the old operator $U(t,s)$ upon exchance of s and t. Therefore all the steps leading to $\subseteq$ in (5.29) yield the desired inclusion $\supseteq$, when applied to the adjoint operator $U_\infty(t_0, t)$. $\square$

6 Estimate of the Rate of Convergence

The object of this chapter is to determine the rate of convergence of $U_\lambda(t, t_0)$ towards $U_\infty(t, t_0)$. In particular, we would like to assess how the error shrinks with growing λ, and which influence is attributed to the time during which the external field interacts with the electron. Physically, one expects the error to be in leading order inversely proportional to the wavelength, as we have truncated the Taylor expansion (2.6) of the field after the zeroth-order term. It is also expectable that the approximation deteriorates in some way with growing time: an external field pumping energy into the system might sooner or later make the electron move out of the regime where the dipole approximation is valid. Note in this context that the kinetic energy of the electron in dipole approximation is uniformly bounded in time, which is not necessarily true for an electron evolving under the exact time evolution.

In Section 4.4, we have argued that it does not make sense to include all possible $L^2(\mathbb{R}^d)$-functions in the estimate of the kinetic energy. The same is the case here: no Coulomb potential could possibly confine an electron corresponding to a wave function with infinite kinetic energy, it would be arbitrarily far away from the nucleus within finite time. For such states, the strongest statement possible is that the convergence happens eventually, but only just in the ultimate limit $\lambda \to \infty$. This was already proved in Theorem 4.1.

For the dipole approximation to be viable for reasonably large λ, we demand that the electron be originally rather localised around the nucleus. As we have seen in Chapter 5, the domain $\mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$ of the harmonic oscillator is left invariant by the time evolution $U_\infty(t, t_0)$. All its elements have finite second and fourth moments in position as well as in momentum (5.28). We will now show that this localisation suffices to achieve an estimate for the rate of convergence.

6.1 Rigorous Result

Theorem 6.1. *Let $\psi \in \mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$. With definitions and assumptions as in Theorem 4.1 and under the additional assumption*

(A5) $\|\partial_j a_i(\cdot, t)\|_\infty \le C < \infty$ uniformly in t for $i, j = 1, \dots, d$,

it holds that

$$\left\| \big(U_\lambda(t, 0) - U_\infty(t, 0)\big)\psi \right\| \le C\, \frac{(1+t)^{\frac{5}{2}}}{\lambda}$$

for some constant C depending on ψ, $\mathbf{a}$, ω and V.

We have included the additional assumption (A5) that the first spatial derivative of the external field be bounded. It can easily be verified that this assumption is fulfilled by the physically relevant examples from Section 4.1.2. Furthermore, we have put $t_0 \equiv 0$ to simplify the notation.

Proof. Since $\mathbf{a}(\cdot, \omega t) \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R}^d)$ for each $t \in [0, T]$, we may express it as a Taylor polynomial with remainder,

$$\mathbf{a}\left(\tfrac{\mathbf{x}}{\lambda}, \omega t\right) = \mathbf{a}\left(0, \omega t\right) + \mathbf{R}_1\left(\tfrac{\mathbf{x}}{\lambda}, \omega t\right).$$

The remainder is given by the Lagrange formula [55, Ch. 2.4] as

$$\mathbf{R}_1\left(\tfrac{\mathbf{x}}{\lambda}, \omega t\right) = \tfrac{1}{\lambda}\sum_{j=1}^{d} \partial_j \mathbf{a}(\xi, \omega t) x_j,$$

for some ξ on the line segment $[0, \frac{\mathbf{x}}{\lambda}]$. After an analogous consideration for $\mathbf{a}\left(\frac{\mathbf{x}}{\lambda}, \omega t\right)^2$, we obtain

$$\mathbf{a}\left(\tfrac{\mathbf{x}}{\lambda}, \omega t\right) - \mathbf{a}\left(0, \omega t\right) = \sum_{j=1}^{d} \partial_j \mathbf{a}(\xi, \omega t) \tfrac{x_j}{\lambda} \tag{6.1}$$

and

$$\mathbf{a}\left(\tfrac{\mathbf{x}}{\lambda}, \omega t\right)^2 - \mathbf{a}\left(0, \omega t\right)^2 = \sum_{j=1}^{d} \partial_j \left(\mathbf{a}(\xi, \omega t)^2\right) \tfrac{x_j}{\lambda}. \tag{6.2}$$

Let $\psi \in \mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$. As this implies that $\psi \in H^2(\mathbb{R}^d)$, the difference between the exact and the approximated time evolution operator $\left\|\left(U_\lambda(t, t_0) - U_\infty(t, t_0)\right)\psi\right\|$ is given by (4.68) and (4.69).

With (6.1) and (6.2), (4.68) and (4.69) yield

$$\begin{aligned} \left\|\left(U_\lambda(t, t_0) - U_\infty(t, t_0)\right)\psi\right\| \leq & \frac{1}{\omega^2\lambda}\int_{t_0}^{t} ds \left(\int_{\mathbb{R}^d} d\mathbf{x} \left|\sum_{j=1}^{d} x_j \partial_j \mathbf{a}(\xi, \omega s)^2 \psi_s^\infty(\mathbf{x})\right|^2\right)^{\frac{1}{2}} \\ & + \frac{2}{\omega\lambda}\int_{t_0}^{t} ds \left(\int_{\mathbb{R}^d} d\mathbf{x} \left|\sum_{j=1}^{d} x_j \partial_j \mathbf{a}(\xi, \omega s) \cdot \nabla\psi_s^\infty(\mathbf{x})\right|^2\right)^{\frac{1}{2}}. \end{aligned} \tag{6.3}$$

Due to assumption (A5), we can define a constant C_5 by

$$C_5 := \sup_{t\in[0,T]} \max_{1\leq j\leq d} \left\{ \left\|\partial_j \mathbf{a}(\cdot, \omega t)\right\|_\infty, \left\|\partial_j \left(\mathbf{a}(\cdot, \omega t)^2\right)\right\|_\infty \right\} < \infty. \tag{6.4}$$

Furthermore,

$$\left(\sum_{j=1}^{d} |x_j|\right)^2 \leq d^2 \left(\max_{1\leq j\leq d} |x_j|\right)^2 \leq d^2 \mathbf{x}^2. \tag{6.5}$$

Hence with (6.4) and (6.5),

$$\begin{aligned} \left\|\left(U_\lambda(t, t_0) - U_\infty(t, t_0)\right)\psi\right\| \leq & \frac{d}{\omega^2\lambda} C_5 \int_{t_0}^{t} ds \left(\int_{\mathbb{R}^d} d\mathbf{x} |\psi_s^\infty \mathbf{x})|^2 \mathbf{x}^2\right)^{\frac{1}{2}} \\ & + \frac{2d}{\omega\lambda} C_5 \int_{t_0}^{t} ds \left(\int_{\mathbb{R}^d} d\mathbf{x} |\nabla\psi_s^\infty(\mathbf{x})|^2 \mathbf{x}^2\right)^{\frac{1}{2}}. \end{aligned} \tag{6.6}$$

The $d\mathbf{x}$-integral contained in the first term of (6.6) can be written compactly as

$$\int_{\mathbb{R}^d} d\mathbf{x}|\psi_s^\infty(\mathbf{x})|^2\mathbf{x}^2 = \left\langle \psi_s^\infty, \mathbf{x}^2\psi_s^\infty \right\rangle,$$

which is well-defined as $\psi_t^\infty \in \mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$ – we have chosen $\psi \in \mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$, and this set is invariant under the time evolution as shown in Theorem 5.4. Hence $\mathbf{x}^2\psi_s^\infty \in L^2(\mathbb{R}^d)$. As argued in Section 5.2, it is impossible to proceed analogously with the corresponding $d\mathbf{x}$-integral in the second term, for $\mathbf{x}^2\partial_j\psi_s^\infty$ is not necessarily an element of $L^2(\mathbb{R}^d)$. We will therefore take again the detour via the bounded operator F_ε.

We need to estimate the expression

$$\left\|\big(U_\lambda(t,t_0) - U_\infty(t,t_0)\big)\psi\right\| \leq \frac{d\,C_5}{\omega^2\lambda}\int_{t_0}^{t} ds\left\langle \psi_s^\infty, \mathbf{x}^2\psi_s^\infty \right\rangle^{\frac{1}{2}} \tag{6.7}$$

$$+\frac{2d\,C_5}{\omega\lambda}\int_{t_0}^{t} ds\left(\int_{\mathbb{R}^d} d\mathbf{x}|\nabla\psi_s^\infty(\mathbf{x})|^2\mathbf{x}^2\right)^{\frac{1}{2}}. \tag{6.8}$$

In the following, we will examine (6.7) and (6.8) separately.

Estimate of (6.7). Let $\psi \in \mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$ and $t \in [0,T]$. Then, as a consequence of the Schrödinger equation,

$$\begin{aligned}\tfrac{d}{dt}\langle \psi_t^\infty, \mathbf{x}^2\psi_t^\infty\rangle &= i\left\langle H_\infty(t)\psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle - i\left\langle \mathbf{x}^2\psi_t^\infty, H_\infty(t)\psi_t^\infty\right\rangle \\ &= i\Big(\left\langle \mathbf{p}^2\psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle - \left\langle \mathbf{x}^2\psi_t^\infty, \mathbf{p}^2\psi_t^\infty\right\rangle\Big) \\ &\quad - \tfrac{2i}{\omega}\Big(\left\langle \mathbf{a}(0,\omega t)\cdot\mathbf{p}\psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle - \left\langle \mathbf{x}^2\psi_t^\infty, \mathbf{a}(0,\omega t)\cdot\mathbf{p}\psi_t^\infty\right\rangle\Big).\end{aligned} \tag{6.9}$$

Formally, this can be evaluated as

$$\begin{aligned}\tfrac{d}{dt}\langle \psi_t^\infty, \mathbf{x}^2\psi_t^\infty\rangle &= i\left\langle \psi_t^\infty, [H_\infty(t), \mathbf{x}^2]\psi_t^\infty\right\rangle \\ &= 2\left\langle \psi_t^\infty, \{\mathbf{p},\mathbf{x}\}\psi_t^\infty\right\rangle - \tfrac{4}{\omega}\left\langle \psi_t^\infty, \mathbf{a}(0,\omega t)\cdot\mathbf{x}\psi_t^\infty\right\rangle,\end{aligned} \tag{6.10}$$

where we have used the commutator

$$[H_\infty(t), \mathbf{x}^2] = -2i\{\mathbf{p},\mathbf{x}\} + \tfrac{4i}{\omega}\mathbf{a}(0,\omega t)\cdot\mathbf{x}.$$

We must however be careful with these operations, as $H_\infty(t)\mathbf{x}^2\psi_t^\infty$ and $\mathbf{x}^2H_\infty(t)\psi_t^\infty$ are not necessarily elements of $L^2(\mathbb{R}^d)$. To render (6.10) rigorous, we make again use of the operator F_ε from Lemma 5.3. From (5.19) and (5.20) we already know that

$$\left\langle \mathbf{p}^2\psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle - \left\langle \mathbf{x}^2\psi_t^\infty, \mathbf{p}^2\psi_t^\infty\right\rangle = -2i\left\langle \psi_t^\infty, \{\mathbf{p},\mathbf{x}\}\psi_t^\infty\right\rangle. \tag{6.11}$$

Proceeding analogously, we compute

$$\begin{aligned}\left\langle \mathbf{a}(0,\omega t)\cdot\mathbf{p}\psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle - \left\langle \mathbf{x}^2\psi_t^\infty, \mathbf{a}(0,\omega t)\cdot\mathbf{p}\psi_t^\infty\right\rangle &= \lim_{\varepsilon\to 0}\left\langle \psi_t^\infty, \mathbf{a}(0,\omega t)\cdot[\mathbf{p},F_\varepsilon]\psi_t^\infty\right\rangle \\ &= -2i\left\langle \psi_t^\infty, \mathbf{a}(0,\omega t)\cdot\mathbf{x}\psi_t^\infty\right\rangle,\end{aligned} \tag{6.12}$$

where we have used that $\langle \psi_t^\infty, [p_j, F_\varepsilon]\psi_t^\infty \rangle$ is bounded uniformly in ε according to Lemma 5.3. Insertion of (6.11) and (6.12) into (6.9) confirms the formal result (6.10). It can be further estimated as

$$\begin{aligned}
\tfrac{d}{dt} \left\langle \psi_t^\infty, \mathbf{x}^2 \psi_t^\infty \right\rangle &= 2 \left\langle \psi_t^\infty, \{\mathbf{p}, \mathbf{x}\} \psi_t^\infty \right\rangle - \tfrac{4}{\omega} \left\langle \psi_t^\infty, \mathbf{a}\,(0, \omega t) \cdot \mathbf{x} \psi_t^\infty \right\rangle \\
&\leq 4 \left\| |\mathbf{p}| \psi_t^\infty \right\| \left\| |\mathbf{x}| \psi_t^\infty \right\| + \tfrac{4}{\omega} C_{\mathbf{a}} \left\| \psi \right\| \left\| |\mathbf{x}| \psi_t^\infty \right\| \\
&= 2 \left\langle \psi_t^\infty, \mathbf{x}^2 \psi_t^\infty \right\rangle^{\frac{1}{2}} \Big(2 \left\| \nabla \psi_t^\infty \right\| + \tfrac{2}{\omega} C_{\mathbf{a}} \left\| \psi \right\| \Big),
\end{aligned}$$

with $C_{\mathbf{a}}$ defined as in (4.24). Thus

$$\tfrac{d}{dt} \Big(\left\langle \psi_t^\infty, \mathbf{x}^2 \psi_t^\infty \right\rangle^{\frac{1}{2}} \Big) \leq 2 \left\| \nabla \psi_t^\infty \right\| + \tfrac{2}{\omega} C_{\mathbf{a}} \left\| \psi \right\|,$$

and accordingly

$$\left\langle \psi_t^\infty, \mathbf{x}^2 \psi_t^\infty \right\rangle^{\frac{1}{2}} \leq \left\langle \psi, \mathbf{x}^2 \psi \right\rangle^{\frac{1}{2}} + 2 \int_{t_0}^{t} \left\| \nabla \psi_s^\infty \right\| ds + \tfrac{2}{\omega} C_{\mathbf{a}} \left\| \psi \right\| (t - t_0). \tag{6.13}$$

This is a consequence of the monotonicity of the integral. As ψ_t^∞ is the wave function evolving under the time evolution generated by the Hamiltonian in dipole approximation, we can use the result of Lemma 4.8,

$$\left\| \nabla \psi_t^\infty \right\| \leq C_4 \left(\left\| \nabla \psi \right\| + \left\| \psi \right\| \right), \tag{6.14}$$

with C_4 defined as in (4.65). Insertion of (6.14) into (6.13) yields

$$\left\langle \psi_t^\infty, \mathbf{x}^2 \psi_t^\infty \right\rangle^{\frac{1}{2}} \leq \left\langle \psi, \mathbf{x}^2 \psi \right\rangle^{\frac{1}{2}} + 2 C_4 \left(\left\| \nabla \psi \right\| + \left(1 + \frac{C_{\mathbf{a}}}{\omega C_4} \right) \left\| \psi \right\| \right) (t - t_0). \tag{6.15}$$

With the abbreviation

$$\alpha_{\omega, \mathbf{a}, V}(\psi) := C_4 \left(\left\| \nabla \psi \right\| + \left(1 + \frac{C_{\mathbf{a}}}{\omega C_4} \right) \left\| \psi \right\| \right), \tag{6.16}$$

this can be written compactly as

$$\left\langle \psi_t^\infty, \mathbf{x}^2 \psi_t^\infty \right\rangle^{\frac{1}{2}} \leq \left\langle \psi, \mathbf{x}^2 \psi \right\rangle^{\frac{1}{2}} + 2 \alpha_{\omega, \mathbf{a}, V}(\psi)(t - t_0). \tag{6.17}$$

Hence (6.7) has the upper bound

$$(6.7) \leq \frac{d\, C_5}{\omega^2 \lambda} \left[\left\langle \psi, \mathbf{x}^2 \psi \right\rangle^{\frac{1}{2}} (t - t_0) + 2 \alpha_{\omega, \mathbf{a}, V}(\psi) \left(\frac{t^2}{2} - \frac{3 t_0^2}{2} - t\, t_0 \right) \right],$$

which for $t_0 = 0$ simplifies to

$$(6.7) \leq \frac{d\, C_5}{\omega^2 \lambda} \Big(\left\langle \psi, \mathbf{x}^2 \psi \right\rangle^{\frac{1}{2}} t + \alpha_{\omega, \mathbf{a}, V}(\psi)\, t^2 \Big). \tag{6.18}$$

Estimate of (6.8). In Section 5.2, we have already proved that

$$\int_{\mathbb{R}^d} |\nabla\psi_t^\infty(\mathbf{x})|^2\mathbf{x}^2 d\mathbf{x} \leq \|-\Delta\psi_t^\infty\| \left\|\mathbf{x}^2\psi_t^\infty\right\| + 2\,\|\nabla\psi_t^\infty\| \left\langle \psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle^{\frac{1}{2}} \tag{6.19}$$

((5.10) to (5.15)). The only unknown quantity in (6.19) is $\left\|\mathbf{x}^2\psi_t^\infty\right\|$, of which we only know that it exists as $\psi_t^\infty \in \mathcal{D}(\mathbf{x}^2)$. Thus an estimate of this will be our next step.

Formally, we compute analogously to the estimate of $\left\langle \psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle$

$$\begin{aligned}
\tfrac{d}{dt}\left\langle \psi_t^\infty, \mathbf{x}^4\psi_t^\infty\right\rangle &= i\left\langle \psi_t^\infty, [H_\infty(t), \mathbf{x}^4]\psi_t^\infty\right\rangle \\
&= 4\left\langle \psi_t^\infty, \{\mathbf{p}, \mathbf{x}^3\}\psi_t^\infty\right\rangle - \tfrac{8}{\omega}\left\langle \psi_t^\infty, \mathbf{a}\,(0,\omega t)\cdot \mathbf{x}^3\psi_t^\infty\right\rangle \\
&\leq 8\,\|\mathbf{x}\cdot\mathbf{p}\psi_t^\infty\| \left\langle \psi_t^\infty, \mathbf{x}^4\psi_t^\infty\right\rangle^{\frac{1}{2}} + \tfrac{8}{\omega}C_{\mathbf{a}}\left\langle \psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle^{\frac{1}{2}}\left\langle \psi_t^\infty, \mathbf{x}^4\psi_t^\infty\right\rangle^{\frac{1}{2}} \\
&\leq \left\langle \psi_t^\infty, \mathbf{x}^4\psi_t^\infty\right\rangle^{\frac{1}{2}}\Bigg(8\left(\left\|\mathbf{p}^2\psi_t^\infty\right\|\left\langle \psi_t^\infty, \mathbf{x}^4\psi_t^\infty\right\rangle^{\frac{1}{2}} + 2\,\||\mathbf{p}|\psi_t^\infty\|\left\langle \psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle^{\frac{1}{2}}\right)^{\frac{1}{2}} \\
&\qquad\qquad + \tfrac{8}{\omega}C_{\mathbf{a}}\left\langle \psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle^{\frac{1}{2}}\Bigg) \\
&\leq \left\langle \psi_t^\infty, (1+\mathbf{x}^4)\psi_t^\infty\right\rangle^{\frac{3}{4}}\left(8\left(\|-\Delta\psi_t^\infty\| + 2\,\|\nabla\psi_t^\infty\|\right)^{\frac{1}{2}} + \tfrac{8}{\omega}C_{\mathbf{a}}\left\langle \psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle^{\frac{1}{4}}\right),
\end{aligned}$$

where we have used the commutator

$$[H_\infty(t), \mathbf{x}^4] = -4i\{\mathbf{p}, \mathbf{x}^3\} + \tfrac{8i}{\omega}\mathbf{a}\,(0,\omega t)\cdot\mathbf{x}^3$$

as well as

$$\left\langle \psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle \leq \left\langle \psi_t^\infty, (1+\mathbf{x}^4)\psi_t^\infty\right\rangle \quad \text{and} \quad \left\langle \psi_t^\infty, \mathbf{x}^4\psi_t^\infty\right\rangle \leq \left\langle \psi_t^\infty, (1+\mathbf{x}^4)\psi_t^\infty\right\rangle.$$

This must however be taken with a grain of salt, as $\mathbf{x}^4\psi_t^\infty$ is not necessarily an element of $L^2(\mathbb{R}^d)$ and hence the scalar product is possibly not well defined. Therefore, we use again the auxiliary operator F_ε. Noting that F_ε^2 maps elements from $H^1(\mathbb{R}^d)$ to $H^1(\mathbb{R}^d)$ and that

$$\left\langle \psi_t^\infty, F_\varepsilon^2\psi_t^\infty\right\rangle \leq \left\|\mathbf{x}^2\psi_t^\infty\right\|^2 < \infty$$

is bounded uniformly in ε as $\psi_t^\infty \in \mathcal{D}(\mathbf{x}^2+\mathbf{p}^2)$, we compute

$$\begin{aligned}
\tfrac{d}{dt}\left\langle \psi_t^\infty, F_\varepsilon^2\psi_t^\infty\right\rangle &= i\left\langle H_\infty(t)\psi_t^\infty, F_\varepsilon^2\psi_t^\infty\right\rangle - i\left\langle F_\varepsilon^2\psi_t^\infty, H_\infty(t)\psi_t^\infty\right\rangle \\
&= i\Big(\left\langle \mathbf{p}^2\psi_t^\infty, F_\varepsilon^2\psi_t^\infty\right\rangle - \left\langle F_\varepsilon^2\psi_t^\infty, \mathbf{p}^2\psi_t^\infty\right\rangle\Big) \\
&\quad - \tfrac{2i}{\omega}\Big(\left\langle \mathbf{a}\,(0,\omega t)\cdot\mathbf{p}\psi_t^\infty, F_\varepsilon^2\psi_t^\infty\right\rangle - \left\langle F_\varepsilon^2\psi_t^\infty, \mathbf{a}\,(0,\omega t)\cdot\mathbf{p}\psi_t^\infty\right\rangle\Big).
\end{aligned}$$

We evaluate separately

$$\begin{aligned}
\left\langle \mathbf{p}^2\psi_t^\infty, F_\varepsilon^2\psi_t^\infty\right\rangle - \left\langle F_\varepsilon^2\psi_t^\infty, \mathbf{p}^2\psi_t^\infty\right\rangle &= \left\langle \mathbf{p}\psi_t^\infty, [\mathbf{p}, F_\varepsilon^2]\psi_t^\infty\right\rangle + \left\langle \psi_t^\infty, [\mathbf{p}, F_\varepsilon^2]\cdot\mathbf{p}\psi_t^\infty\right\rangle \\
&= -2i\Big(\langle \psi_t^\infty, \mathbf{p}\cdot(\nabla F_\varepsilon)F_\varepsilon\psi_t^\infty\rangle + \langle \psi_t^\infty, F_\varepsilon(\nabla F_\varepsilon)\cdot\mathbf{p}\psi_t^\infty\rangle\Big)
\end{aligned}$$

and

$$\left\langle \mathbf{a}\,(0,\omega t)\cdot\mathbf{p}\psi_t^\infty, F_\varepsilon^2\psi_t^\infty\right\rangle - \left\langle F_\varepsilon^2\psi_t^\infty, \mathbf{a}\,(0,\omega t)\cdot\mathbf{p}\psi_t^\infty\right\rangle = \left\langle \psi_t^\infty, \mathbf{a}\,(0,\omega t)\cdot[\mathbf{p}, F_\varepsilon^2]\psi_t^\infty\right\rangle$$
$$= -2i\,\langle \psi_t^\infty, \mathbf{a}\,(0,\omega t)\cdot(\nabla F_\varepsilon)F_\varepsilon\psi_t^\infty\rangle\,.$$

Here, ∇F_ε denotes the multiplication operator corresponding to the gradient

$$\nabla F_\varepsilon(\mathbf{x}) = \frac{2\mathbf{x}}{(1+\varepsilon\mathbf{x}^2)^2}\ , \tag{6.20}$$

which is, according to Lemma 5.3, symmetric and bounded from $H^1(\mathbb{R}^d)$ to $H^1(\mathbb{R}^d)$. Hence

$$\begin{aligned}
\tfrac{d}{dt}\,\|F_\varepsilon\psi_t^\infty\|^2 &= \tfrac{d}{dt}\langle\psi_t^\infty, F_\varepsilon^2\psi_t^\infty\rangle\\
&= 2\,\langle\psi_t^\infty, \mathbf{p}\cdot(\nabla F_\varepsilon)F_\varepsilon\psi_t^\infty\rangle + 2\,\langle\psi_t^\infty, F_\varepsilon(\nabla F_\varepsilon)\cdot\mathbf{p}\psi_t^\infty\rangle\\
&\quad - \tfrac{4}{\omega}\,\langle\psi_t^\infty, \mathbf{a}\,(0,\omega t)\cdot(\nabla F_\varepsilon)F_\varepsilon\psi_t^\infty\rangle\\
&\le 4\,\|F_\varepsilon\psi_t^\infty\|\,\|(\nabla F_\varepsilon)\cdot\mathbf{p}\psi_t^\infty\| + \tfrac{4}{\omega}C_{\mathbf{a}}\,\||\nabla F_\varepsilon|\psi_t^\infty\|\,\|F_\varepsilon\psi_t^\infty\|\\
&= 4\left\langle\psi_t^\infty, F_\varepsilon^2\psi_t^\infty\right\rangle^{\frac12}\Big(\,\|(\nabla F_\varepsilon)\cdot\mathbf{p}\psi_t^\infty\| + \tfrac{C_{\mathbf{a}}}{\omega}\,\||\nabla F_\varepsilon|\psi_t^\infty\|\,\Big).
\end{aligned} \tag{6.21}$$

With (6.20), the second term within the brackets in (6.21) can be estimated as

$$\||\nabla F_\varepsilon|\psi_t^\infty\|^2 = \int_{\mathbb{R}^d}\frac{4\mathbf{x}^2}{(1+\varepsilon\mathbf{x}^2)^4}|\psi_t^\infty(\mathbf{x})|^2 d\mathbf{x} \le 4\,\langle\psi_t^\infty, F_\varepsilon\psi_t^\infty\rangle\,. \tag{6.22}$$

For the first term, we apply the Cauchy-Schwarz inequality in the Euclidean scalar product and obtain analogously

$$\begin{aligned}
\|(\nabla F_\varepsilon)\cdot\mathbf{p}\psi_t^\infty\|^2 &\le 4\int_{\mathbb{R}^d} F_\varepsilon(\mathbf{x})|\nabla\psi_t^\infty(\mathbf{x})|^2 d\mathbf{x}\\
&\le 4\left\|\mathbf{p}^2\psi_t^\infty\right\|\,\|F_\varepsilon\psi_t^\infty\| + 8\,\||\mathbf{p}|\psi_t^\infty\|\,\langle\psi_t^\infty, F_\varepsilon\psi_t^\infty\rangle^{\frac12}\,,
\end{aligned} \tag{6.23}$$

where we have made use of (5.12). Insertion of (6.22) and (6.23) into (6.21) yields

$$\begin{aligned}
&\tfrac{d}{dt}\langle\psi_t^\infty, F_\varepsilon^2\psi_t^\infty\rangle\\
&\quad\le 4\left\langle\psi_t^\infty, F_\varepsilon^2\psi_t^\infty\right\rangle^{\frac12}\Bigg(\Big(4\,\|-\Delta\psi_t^\infty\|\,\langle\psi_t^\infty, F_\varepsilon^2\psi_t^\infty\rangle^{\frac12} + 8\,\|\nabla\psi_t^\infty\|\,\langle\psi_t^\infty, F_\varepsilon\psi_t^\infty\rangle^{\frac12}\Big)^{\frac12}\\
&\qquad\qquad + \tfrac{2}{\omega}C_{\mathbf{a}}\,\langle\psi_t^\infty, F_\varepsilon\psi_t^\infty\rangle^{\frac12}\Bigg)\\
&\quad\le 4\left\langle\psi_t^\infty, (1+F_\varepsilon^2)\psi_t^\infty\right\rangle^{\frac34}\Big(2\,(\|-\Delta\psi_t^\infty\| + 2\,\|\nabla\psi_t^\infty\|)^{\frac12} + \tfrac{2}{\omega}C_{\mathbf{a}}\,\langle\psi_t^\infty, F_\varepsilon\psi_t^\infty\rangle^{\frac14}\Big)
\end{aligned}$$

analogously to the formal consideration. Observing that

$$\tfrac{d}{dt}\left\langle\psi_t^\infty, F_\varepsilon^2\psi_t^\infty\right\rangle = \tfrac{d}{dt}\left\langle\psi_t^\infty, (1+F_\varepsilon^2)\psi_t^\infty\right\rangle$$

due to the unitarity of the time evolution, we infer

$$\tfrac{d}{dt}\Big(\left\langle\psi_t^\infty, (1+F_\varepsilon^2)\psi_t^\infty\right\rangle^{\frac14}\Big) \le 2\big(\,\|-\Delta\psi_t^\infty\| + 2\,\|\nabla\psi_t^\infty\|\,\big)^{\frac12} + \tfrac{2}{\omega}C_{\mathbf{a}}\,\langle\psi_t^\infty, F_\varepsilon\psi_t^\infty\rangle^{\frac14}\,,$$

and accordingly

$$\left\langle \psi_t^\infty, (1+F_\varepsilon^2)\psi_t^\infty \right\rangle^{\frac{1}{4}} \leq \left\langle \psi, (1+F_\varepsilon^2)\psi \right\rangle^{\frac{1}{4}} + 2\int_{t_0}^{t} \left(\|-\Delta\psi_s^\infty\| + 2\,\|\nabla\psi_s^\infty\| \right)^{\frac{1}{2}} ds + \tfrac{2}{\omega} C_{\mathbf{a}} \int_{t_0}^{t} \langle \psi_s^\infty, F_\varepsilon \psi_s^\infty \rangle^{\frac{1}{4}}\, ds.$$

Thus

$$\|F_\varepsilon \psi_t^\infty\| \leq \left(\left(\|\psi\| + \|F_\varepsilon\psi\| \right)^{\frac{1}{2}} + 2\int_{t_0}^{t} \left(\|-\Delta\psi_s^\infty\| + 2\,\|\nabla\psi_s^\infty\| \right)^{\frac{1}{2}} ds + \tfrac{2}{\omega} C_{\mathbf{a}} \int_{t_0}^{t} \langle \psi_s^\infty, F_\varepsilon \psi_s^\infty \rangle^{\frac{1}{4}}\, ds \right)^2, \tag{6.24}$$

where we have used that

$$\left\langle \psi_t^\infty, F_\varepsilon^2 \psi_t^\infty \right\rangle \leq \left\langle \psi_t^\infty, (1+F_\varepsilon^2)\psi_t^\infty \right\rangle \leq \left(\|\psi\| + \|F_\varepsilon\psi\| \right)^2.$$

All terms being bounded uniformly in ε, we may apply the theorem of dominated convergence to (6.24) and conclude

$$\left\|\mathbf{x}^2\psi_t^\infty\right\| \leq \left(\left(\|\psi\| + \left\|\mathbf{x}^2\psi\right\| \right)^{\frac{1}{2}} + 2\int_{t_0}^{t} \left(\|-\Delta\psi\| + 2\,\|\nabla\psi\| \right)^{\frac{1}{2}} + \tfrac{2}{\omega} C_{\mathbf{a}} \int_{t_0}^{t} \left\langle \psi_s^\infty, \mathbf{x}^2 \psi_s^\infty \right\rangle^{\frac{1}{4}}\, ds \right)^2. \tag{6.25}$$

With the aid of Lemma 4.8, we estimate

$$\left(\|-\Delta\psi_t^\infty\| + 2\,\|\nabla\psi_t^\infty\| \right)^{\frac{1}{2}} \leq \beta_V(\psi),$$

where we have introduced the abbreviation

$$\beta_V(\psi) := C_4^{\frac{1}{2}} \left(\|-\Delta\psi\| + 2\,\|\nabla\psi\| + 3\,\|\psi\| \right)^{\frac{1}{2}}. \tag{6.26}$$

For simplicity, we consider in the following only the case $t_0 = 0$. Then (6.25) yields

$$\begin{aligned}
\left\|\mathbf{x}^2\psi_t^\infty\right\| &\leq \left(\left(\|\psi\| + \left\|\mathbf{x}^2\psi\right\| \right)^{\frac{1}{2}} + 2\beta_V(\psi)t + \tfrac{2}{\omega} C_{\mathbf{a}} \int_0^t \left(\left\langle \psi, \mathbf{x}^2\psi \right\rangle^{\frac{1}{2}} + 2\alpha_{\omega,\mathbf{a},V}(\psi)s \right)^{\frac{1}{2}} ds \right)^2 \\
&= \left(\left(\|\psi\| + \left\|\mathbf{x}^2\psi\right\| \right)^{\frac{1}{2}} + 2\beta_V(\psi)t + \frac{2C_{\mathbf{a}}}{3\omega\, \alpha_{\omega,\mathbf{a},V}(\psi)} \left[\left(\left\langle \psi, \mathbf{x}^2\psi \right\rangle^{\frac{1}{2}} + 2\alpha_{\omega,\mathbf{a},V}(\psi)\, t \right)^{\frac{3}{2}} - \left\langle \psi, \mathbf{x}^2\psi \right\rangle^{\frac{3}{4}} \right] \right)^2 \\
&\leq \left(\left(\|\psi\| + \left\|\mathbf{x}^2\psi\right\| \right)^{\frac{1}{2}} + 2\beta_V(\psi)t + \gamma_{\omega,\mathbf{a},V}(\psi) \left(\left\langle \psi, \mathbf{x}^2\psi \right\rangle^{\frac{1}{2}} + 2\alpha_{\omega,\mathbf{a},V}(\psi)\, t \right)^{\frac{3}{2}} \right)^2,
\end{aligned}$$

with $\alpha_{\omega,\mathbf{a},V}(\psi)$ as in (6.16) and with the abbreviation

$$\gamma_{\omega,\mathbf{a},V}(\psi) := \frac{2C_{\mathbf{a}}}{3\omega\alpha_{\omega,\mathbf{a},V}(\psi)}. \tag{6.27}$$

This can be further evaluated as

$$\begin{aligned}
\left\|\mathbf{x}^2\psi_t^\infty\right\| \leq \|\psi\| + \left\|\mathbf{x}^2\psi\right\| & \\
+ 4\left(\|\psi\| + \left\|\mathbf{x}^2\psi\right\|\right)^{\frac{1}{2}} \beta_V(\psi)\, t & \\
+ \left(\|\psi\| + \left\|\mathbf{x}^2\psi\right\|\right)^{\frac{1}{2}} 2\gamma_{\omega,\mathbf{a},V}(\psi) \left(\left\langle\psi, \mathbf{x}^2\psi\right\rangle^{\frac{1}{2}} + 2\alpha_{\omega,\mathbf{a},V}(\psi)\, t\right)^{\frac{3}{2}} & \\
+ 4\beta_V(\psi)^2\, t^2 & \\
+ 4\gamma_{\omega,\mathbf{a},V}(\psi)\beta_V(\psi) \left(\left\langle\psi, \mathbf{x}^2\psi\right\rangle^{\frac{1}{2}} + 2\alpha_{\omega,\mathbf{a},V}(\psi)\, t\right)^{\frac{3}{2}} t & \\
+ \gamma_{\omega,\mathbf{a},V}(\psi)^2 \left(\left\langle\psi, \mathbf{x}^2\psi\right\rangle^{\frac{1}{2}} + 2\alpha_{\omega,\mathbf{a},V}(\psi)\, t\right)^3. &
\end{aligned} \tag{6.28}$$

Now we insert (6.17) and (6.26) into (6.19), which yields

$$\begin{aligned}
\int_{\mathbb{R}^d} |\nabla\psi_t^\infty(\mathbf{x})|^2\mathbf{x}^2 d\mathbf{x} &\leq \|-\Delta\psi_t^\infty\| \left\|\mathbf{x}^2\psi_t^\infty\right\| + 2\,\|\nabla\psi_t^\infty\| \left\langle\psi_t^\infty, \mathbf{x}^2\psi_t^\infty\right\rangle^{\frac{1}{2}} \\
&\leq \beta_V(\psi)^2 \left(\left\|\mathbf{x}^2\psi_t^\infty\right\| + \left\langle\psi, \mathbf{x}^2\psi\right\rangle^{\frac{1}{2}} + 2\alpha_{\omega,\mathbf{a},V}(\psi)\, t\right).
\end{aligned}$$

Estimating

$$\begin{aligned}
\left(\left\langle\psi, \mathbf{x}^2\psi\right\rangle^{\frac{1}{2}} + 2\alpha_{\omega,\mathbf{a},V}(\psi)\, t\right)^{\frac{3}{2}} &\leq 1 + \left(\left\langle\psi, \mathbf{x}^2\psi\right\rangle^{\frac{1}{2}} + 2\alpha_{\omega,\mathbf{a},V}(\psi)\, t\right)^2 \\
&= 1 + \left\langle\psi, \mathbf{x}^2\psi\right\rangle + 4\left\langle\psi, \mathbf{x}^2\psi\right\rangle^{\frac{1}{2}} \alpha_{\omega,\mathbf{a},V}(\psi)\, t + 4\alpha_{\omega,\mathbf{a},V}(\psi)^2\, t^2
\end{aligned}$$

and expanding the last term in (6.28), we obtain

$$\int_{\mathbb{R}^d} |\nabla\psi_t^\infty(\mathbf{x})|^2\mathbf{x}^2 d\mathbf{x} \leq \beta_V(\psi)^2\big(\delta_{\omega,\mathbf{a},V}(\psi) + \varepsilon_{\omega,\mathbf{a},V}(\psi)t + \zeta_{\omega,\mathbf{a},V}(\psi)t^2 + \eta_{\omega,\mathbf{a},V}(\psi)t^3\big),$$

where

$$\begin{aligned}
\delta_{\omega,\mathbf{a},V}(\psi) &:= \|\psi\| + \left\|\mathbf{x}^2\psi\right\| + 2\gamma_{\omega,\mathbf{a},V}(\psi) \left(\|\psi\| + \left\|\mathbf{x}^2\psi\right\|\right)^{\frac{1}{2}} \left(1 + \left\langle\psi, \mathbf{x}^2\psi\right\rangle\right) + \left\langle\psi, \mathbf{x}^2\psi\right\rangle^{\frac{1}{2}} \\
&\quad + \gamma_{\omega,\mathbf{a},V}(\psi)^2 \left\langle\psi, \mathbf{x}^2\psi\right\rangle^{\frac{3}{2}}, \\
\varepsilon_{\omega,\mathbf{a},V}(\psi) &:= 2\alpha_{\omega,\mathbf{a},V}(\psi) + 4\beta_V(\psi)\gamma_{\omega,\mathbf{a},V}(\psi) \\
&\quad + 2\left\langle\psi, \mathbf{x}^2\psi\right\rangle \left(2\gamma_{\omega,\mathbf{a},V}(\psi)\beta_V(\psi) + 3\alpha_{\omega,\mathbf{a},V}(\psi)\gamma_{\omega,\mathbf{a},V}(\psi)^2\right) \\
&\quad + 4\left(\|\psi\| + \left\|\mathbf{x}^2\psi\right\|\right)^{\frac{1}{2}} \left(\beta_V(\psi) + 2\left\langle\psi, \mathbf{x}^2\psi\right\rangle^{\frac{1}{2}} \alpha_{\omega,\mathbf{a},V}(\psi)\gamma_{\omega,\mathbf{a},V}(\psi)\right), \\
\zeta_{\omega,\mathbf{a},V}(\psi) &:= 4\beta_V(\psi)^2 + 8\left(\|\psi\| + \left\|\mathbf{x}^2\psi\right\|\right)^{\frac{1}{2}} \gamma_{\omega,\mathbf{a},V}(\psi)\alpha_{\omega,\mathbf{a},V}(\psi)^2 \\
&\quad + 4\left\langle\psi, \mathbf{x}^2\psi\right\rangle^{\frac{1}{2}} \alpha_{\omega,\mathbf{a},V}(\psi)\gamma_{\omega,\mathbf{a},V}(\psi)\Big(4\beta_V(\psi) + 3\alpha_{\omega,\mathbf{a},V}(\psi)\gamma_{\omega,\mathbf{a},V}(\psi)\Big), \\
\eta_{\omega,\mathbf{a},V}(\psi) &:= 8\alpha_{\omega,\mathbf{a},V}(\psi)^2\gamma_{\omega,\mathbf{a},V}(\psi)\Big(2\beta_V(\psi) + \alpha_{\omega,\mathbf{a},V}(\psi)\gamma_{\omega,\mathbf{a},V}(\psi)\Big).
\end{aligned}$$

Thus

$$
\begin{aligned}
(6.8) &\leq \frac{2dC_5}{\omega\lambda}\beta_V(\psi)\int\limits_0^t \Big(\delta_{\omega,\mathbf{a},V}(\psi)+\varepsilon_{\omega,\mathbf{a},V}(\psi)\,s+\zeta_{\omega,\mathbf{a},V}(\psi)\,s^2+\eta_{\omega,\mathbf{a},V}(\psi)\,s^3\Big)^{\frac{1}{2}}ds \\
&=: \frac{2dC_5}{\omega\lambda}\beta_V(\psi)F(t).
\end{aligned}
\tag{6.29}
$$

The integral in (6.29) can be evaluated exactly. Its solution is however extremely long, and as the explicit form does not provide any deeper insight we refrain from exposing it here. It suffices to note that the solution $F(t)$ is clearly a continuous function.

We finally obtain the rate of convergence for $\psi \in \mathcal{D}(\mathbf{x}^2+\mathbf{p}^2)$ as

$$
\big\|\big(U_\lambda(t,t_0)-U_\infty(t,t_0)\big)\psi\big\| \leq \frac{dC_4}{\omega}\left[\frac{1}{\omega}\Big(\langle\psi,\mathbf{x}^2\psi\rangle^{\frac{1}{2}}\,t+\alpha_{\omega,\mathbf{a},V}(\psi)t^2\Big)+2\beta_V(\psi)F(t)\right]\frac{1}{\lambda}.
$$

To convey a sense of its behaviour, we estimate the integrand in (6.29) very roughly by its leading order term $\sim t^{3/2}$: observing that

$$
s \leq 1+s^3 \text{ and } s^2 \leq 1+s^3 \text{ for } s \geq 0
$$

and

$$
(a+bs^3)^{\frac{1}{2}} \leq \Big(a^{\frac{1}{3}}+b^{\frac{1}{3}}s\Big)^{\frac{3}{2}} \text{ for } a,b,s \geq 0,
$$

we estimate the integral in (6.29) as

$$
\begin{aligned}
&\int\limits_0^t \Big(\big(\delta_{\omega,\mathbf{a},V}(\psi)+\varepsilon_{\omega,\mathbf{a},V}(\psi)+\zeta_{\omega,\mathbf{a},V}(\psi)\big)+\big(\varepsilon_{\omega,\mathbf{a},V}(\psi)+\zeta_{\omega,\mathbf{a},V}(\psi)+\eta_{\omega,\mathbf{a},V}(\psi)\big)\,s^3\Big)^{\frac{1}{2}}ds \\
&\quad\leq \int\limits_0^t \Big(\big(\delta_{\omega,\mathbf{a},V}(\psi)+\varepsilon_{\omega,\mathbf{a},V}(\psi)+\zeta_{\omega,\mathbf{a},V}(\psi)\big)^{\frac{1}{3}}+\big(\varepsilon_{\omega,\mathbf{a},V}(\psi)+\zeta_{\omega,\mathbf{a},V}(\psi)+\eta_{\omega,\mathbf{a},V}(\psi)\big)^{\frac{1}{3}}\,s\Big)^{\frac{3}{2}}ds \\
&\quad= \frac{2}{5}\big(\varepsilon_{\omega,\mathbf{a},V}(\psi)+\zeta_{\omega,\mathbf{a},V}(\psi)+\eta_{\omega,\mathbf{a},V}(\psi)\big)^{-\frac{1}{3}}\;\cdot \\
&\qquad\cdot\Big(\big(\delta_{\omega,\mathbf{a},V}(\psi)+\varepsilon_{\omega,\mathbf{a},V}(\psi)+\zeta_{\omega,\mathbf{a},V}(\psi)\big)^{\frac{1}{3}}+\big(\varepsilon_{\omega,\mathbf{a},V}(\psi)+\zeta_{\omega,\mathbf{a},V}(\psi)+\eta_{\omega,\mathbf{a},V}(\psi)\big)^{\frac{1}{3}}\,t\Big)^{\frac{5}{2}} \\
&\quad\leq \frac{2}{5}\left(\frac{\big(\delta_{\omega,\mathbf{a},V}(\psi)+\varepsilon_{\omega,\mathbf{a},V}(\psi)+\zeta_{\omega,\mathbf{a},V}(\psi)+\eta_{\omega,\mathbf{a},V}(\psi)\big)^{\frac{5}{2}}}{\varepsilon_{\omega,\mathbf{a},V}(\psi)+\zeta_{\omega,\mathbf{a},V}(\psi)+\eta_{\omega,\mathbf{a},V}(\psi)}\right)^{\frac{1}{3}}(1+t)^{\frac{5}{2}},
\end{aligned}
$$

hence $F(t)$ is of leading order $t^{5/2}$. In particular, we conclude

$$
\big\|\big(U_\lambda(t,t_0)-U_\infty(t,t_0)\big)\psi\big\| \leq C(\psi,\omega,\mathbf{a},V)\frac{(1+t)^{\frac{5}{2}}}{\lambda},
$$

where $C(\psi,\omega,\mathbf{a},V)$ is some constant depending on the initial wave function ψ, the external field $\mathbf{a}$, its frequency ω and the potential V. $\square$

For sufficiently large t (in particular $t \geq 1$) we find as a consequence of Theorem 6.1 that

$$\left\| \big(U_\lambda(t,t_0) - U_\infty(t,t_0)\big)\psi \right\| \leq C(\psi, \mathbf{a}, \omega) \frac{(1+t)^{\frac{5}{2}}}{\lambda} \sim \frac{t^{\frac{5}{2}}}{\lambda}.$$

We have thus recovered the expected dependence on $\frac{1}{\lambda}$ and seen that the error grows with the time during which the external field is switched on. The proportionality constant depends on the initial wave function: on its initial localisation, in particular on $\|\psi\|$, $\langle \psi, \mathbf{x}^2\psi \rangle$ and $\langle \psi, \mathbf{x}^4\psi \rangle$, and on its initial regularity, in particular on $\|\nabla\psi\|$ and $\|-\Delta\psi\|$. The other contributing factors are parameters of the external field: its frequency and amplitude as well as its time and spatial derivatives. The choice of the atomic potential enters through the constant C_4, which comprises the coefficients of infinitesimal boundedness of V.

6.2 Effective Bounds

We could now try to transfer this mathematical result to experimental reality by calculating numerical values for $\delta_{\omega,\mathbf{a},V}(\psi)$, $\varepsilon_{\omega,\mathbf{a},V}(\psi)$, $\zeta_{\omega,\mathbf{a},V}(\psi)$ and $\eta_{\omega,\mathbf{a},V}(\psi)$ for relevant initial wave functions ψ. While this certainly demands lengthy calculations, the resulting constant $C(\psi, \omega, \mathbf{a}, V)$ would not be particularly illuminating. Our analysis was done for the class of wave functions we deem the broadest to permit quantitative estimates at all, the elements of $\mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$. *Real* electrons in *real* laboratories are however *effectively* described by much simpler functions, for instance by elements of $\mathcal{C}_c^\infty(\mathbb{R}^3)$. Although it is mathematically not necessarily true that the support of a $\mathcal{C}_c^\infty(\mathbb{R}^3)$-function remains compact under the time evolution, in practice one might just consider the support to be the whole laboratory and neglect the tiny part of the wave function that might escape. For such functions, our estimates simplify considerably from the very beginning due to the compactness of the support: assume ψ_t^∞ would remain effectively in $\mathcal{C}_c^\infty(\mathbb{R}^3)$ for the time span of an experiment. Then we could find some $R > 0$ such that $\operatorname{supp}(\psi_t^\infty) \subseteq B_R(0)$, and the estimate of (6.3) would reduce to

$$\begin{aligned}
\left\| \big(U_\lambda(t,0) - U_\infty(t,0)\big)\psi \right\| &\lesssim \frac{1}{\omega^2\lambda} \int_0^t ds \left(\int_{B_R(0)} d\mathbf{x} \left| \sum_{j=1}^3 R\, \partial_j \mathbf{a}(\xi, \omega s)^2 \psi_s^\infty(\mathbf{x}) \right|^2 \right)^{\frac{1}{2}} \\
&\quad + \frac{2}{\omega\lambda} \int_0^t ds \left(\int_{B_R(0)} d\mathbf{x} \left| \sum_{j=1}^3 R\, \partial_j \mathbf{a}(\xi, \omega s) \cdot \nabla\psi_s^\infty(\mathbf{x}) \right|^2 \right)^{\frac{1}{2}} \\
&\leq \left[\frac{3C_5 R}{\omega^2} \|\psi\| + \frac{6C_4C_5R}{\omega} \left(\|\psi\| + \|\nabla\psi\| \right) \right] \frac{t}{\lambda} \\
&\propto \frac{t}{\lambda},
\end{aligned}$$

which grows merely linearly in t. In fact, one might achieve an even better effective bound as the estimate $|x_i| \leq R$ was not particularly subtle.

Our result of Theorem 6.1 is nevertheless valid as a *rigorous* upper bound on the rate of convergence. For specific wave functions as they may be prepared in a laboratory, it is possible to derive better *effective* bounds – but this was neither the intention nor is it within the scope of this thesis.

7 Conclusion

Under usual experimental conditions, an electron moving in an atomic potential and subject to an external electromagnetic field can be described by a semiclassical Hamiltonian: the electron is treated quantum mechanically, the field classically. If the electronic wave function is localised to a sufficiently small area around the nucleus, one may neglect the spatial variation of the field completely. This simplification is called the *dipole approximation* because the resulting Hamiltonian is gauge equivalent to a Hamiltonian describing the interaction of an electric dipole with a spatially constant electric field.

In this thesis, we have shown that the dipole approximation holds true in the limit of infinite wavelength of the external field, compared to the atomic length scale. To this end, we have proved the self-adjointness of exact and approximated Hamiltonian by an application of the Kato-Rellich theorem. Subsequently, we have established existence, uniqueness and unitarity of the time evolution operators $U_\lambda(t, t_0)$ and $U_\infty(t, t_0)$ generated by the respective Hamiltonians. Two different paths lead to this conclusion: one can either prove the conditions of Kato's theorems or verify the assumptions of a theorem by Yosida. A crucial ingredient for both proofs is the observation that the graph norms of both Hamiltonians are equivalent to the Sobolev norm uniformly in time.
We have derived upper bounds for the kinetic energy of a wave function evolving under $U_\lambda(t, t_0)$ and $U_\infty(t, t_0)$ respectively, the former being exponential and the latter uniform in time. The strong convergence of $U_\lambda(t, t_0)$ towards $U_\infty(t, t_0)$ in the limit of $\lambda, c \to \infty$ has then been established by expressing the difference between $U_\lambda(t, t_0)$ and $U_\infty(t, t_0)$ by the difference between the Hamiltonians, as a consequence of the theorem of dominated convergence.

The second part has been devoted to an estimate of the rate of the convergence. We have argued that such an estimate is not possible for every $L^2(\mathbb{R}^d)$-function, but requires at least a finite kinetic energy and a certain localisation of the time-evolved wave function. Employing Kato's theorem again, we have established the invariance of the domain of the quantum harmonic oscillator under $U_\infty(t, t_0)$. This space ensures finite second and fourth momenta in both position and momentum, which is sufficient for a quantitative analysis. As a side result, we have also proved that the set $\mathcal{C}^\infty(H(t))$ remains unaltered by the time evolution in dipole approximation.
For initial wave functions $\psi \in \mathcal{D}(\mathbf{x}^2 + \mathbf{p}^2)$, we have derived a rigorous upper bound on the error term $\|(U_\lambda(t, t_0) - U_\infty(t, t_0))\psi\|$. To this end, we have expressed the external field by its Taylor polynomial and derived estimates for $\langle \psi, \mathbf{x}^2 \psi \rangle$ and $\langle \psi, \mathbf{x}^4 \psi \rangle$. We have found the rate to be inversely proportional to the wavelength of the external field, and to grow with time as $t^{\frac{5}{2}}$. In particular, the $\frac{1}{\lambda}$-dependence meets the physically motivated expectations; the time-dependence may be improved for specific initial wave functions.

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References

[1] J. J. Sakurai. *Advanced Quantum Mechanics.* Addison-Wesley, 1967.

[2] C. J. Foot. *Atomic Physics.* Oxford University Press, 2005.

[3] W. Demtröder. *Experimentalphysik 3: Atome, Moleküle und Festkörper.* Springer, 2010.

[4] J. Fröhlich, A. Pizzo and B. Schlein. Ionization of Atoms by Intense Laser Pulses. *Annales Henri Poincaré*, 11(7), 2010.

[5] O. Costin, J. L. Lebowitz and C. Stucchio. Ionization in a 1-dimensional dipole model. *Review of Mathematical Physics*, 20(7), 2008.

[6] K. Yajima. Resonance for the AC-Stark effect. *Communications in Mathematical Physics*, 87(3), 1982/83.

[7] S. Graffi and K. Yajima. Exterior Complex Scaling and the AC-Stark effect in a Coulomb field. *Communications in Mathematical Physics*, 89(2), 1983.

[8] J. S. Møller. Two-Body Short-Range Systems in a Time-Periodic Electric Field. *Duke Mathematical Journal*, 105(1), 2000.

[9] W. Pauli and M. Fierz. Zur Theorie der Emission langwelliger Lichtquanten. *Il Nuovo Cimento*, 15(3), 1938.

[10] V. Bach, J. Fröhlich and I. M. Sigal. Quantum Electrodynamics of Confined Nonrelativistic Particles. *Advances in Mathematics*, 137, 1998.

[11] M. Griesemer and H. Zenk. On the Atomic Photoeffect in Non-relativistic QED. *Communications in Mathematical Physics*, 300(3), 2010.

[12] D. Dürr, R. Grummt and M. Kolb. On the Proof of the Dipole Approximation. *arXiv:1309.1655v1 [math-ph]*, September 2013.

[13] R. Grummt. *On Quantum Mechanical Decay Processes.* PhD thesis, 2013.

[14] M. Reed and B. Simon. *Methods of Modern Mathematical Physics Vol. II: Fourier Analysis, Self-Adjointness.* Academic Press, 1975.

[15] T. Kato. Linear evolution equations of “hyperbolic” type. *Journal of the Faculty of Science Univ. of Tokyo Section 1A Mathematics*, 17, 1970.

[16] K. Yosida. *Functional Analysis.* Springer, 1980.

[17] C. Radin and B. Simon. Invariant Domains for the Time-Dependent Schrödinger Equation. *Journal of Differential Equations*, 29(2), August 1978.

[18] M.-J. Huang. Commutators and Invariant Domains for Schrödinger Propagators. *Pacific Journal of Mathematics*, 175(1), 1996.

[19] C. Cohen-Tannoudji, J. Dupont-Roc and G. Grynberg. *Photoms and Atoms – Introduction to Quantum Electrodynamics*. Wiley-VCH, 2004.

[20] C. Cohen-Tannoudji, B. Diu and F. Laloë. *Quantenmechanik, Band 2*. Walter de Gruyter, 2008.

[21] J. D. Jackson. *Klassische Elektrodynamik*. Walter de Gruyter, 2002.

[22] E. C. Kemble. *The Fundamental Principles of Quantum Mechanics – With Elementary Applications*. Dover Publications, 1958.

[23] A. Ludwig et al. Breakdown of the Dipole Approximation in Strong-Field Ionization. *Physical Review Letters*, 113(24), 2014.

[24] D. Dürr and S. Teufel. *Bohmian Mechanics – The Physics and Mathematics of Quantum Theory*. Springer, 2009.

[25] S. Teufel. *Mathematische Physik II – Quantenmechanik*. Lecture at Eberhard Karls Universität Tübingen, Summer term 2016.

[26] M. Reed and B. Simon. *Methods of Modern Mathematical Physics Vol. I: Functional Analysis*. Academic Press, 1975.

[27] G. Teschl. *Mathematical Methods in Quantum Mechanics. With Applications to Schrödinger operators*. American Mathematical Society, 2009.

[28] J. Weidmann. *Lineare Operatoren in Hilberträumen – Teil 1: Grundlagen*. B. G. Teubner, 2000.

[29] P. Müller. *Functional Analysis*. Lecture at Ludwig-Maximilians-Universität München, Summer term 2014.

[30] S. Bachmann. *Mathematical Quantum Mechanics*. Lecture at Ludwig-Maximilians-Universität München, Winter term 2015/16.

[31] R. A. Adams. *Sobolev Spaces*. Academic Press, 1975.

[32] A. Pazy. *Semigroups of Linear Operators and Applications to Partial Differential Equations*. Springer, 1980.

[33] K.-J. Engel and R. Nagel. *One Parameter Semigroups for Linear Evolution Equations*. Springer, 2000.

[34] E. Hille and R. S. Philips. *Functional Analysis and Semi-Groups*. American Mathematical Society, 1957.

[35] J. Schmid. *Adiabatensätze mit und ohne Spektrallückenbedingung*. Master thesis, 2011.

[36] M. Griesemer and J. Schmid. Kato's Theorem on the Integration of Non-Autonomous Linear Evolution Equations. *Mathematical Physics Analysis and Geometry*, 17, 2014.

[37] L. C. Evans. *Partial Differential Equations*. American Mathematical Society, 2010.

[38] B. G. Pachpatte. *Mathematics in science and engineering Vol. 197: Inequalities for differential and integral equations*. Academic Press, 1998.

[39] T. Kato. Integration of the equation of evolution in a Banach space. *Journal of the Mathematical Society of Japan*, 5(2), July 1953.

[40] T. Kato. Linear evolution equations of "hyperbolic" type II. *Journal of the Mathematical Society of Japan*, 25(4), 1973.

[41] T. Kato. *Perturbation Theory of Linear Operators*. Springer, 1995.

[42] E. Heyn. Die Differentialgleichung $\frac{dT}{dt} = P(t)T$ für Operatorfunktionen. *Mathematische Nachrichten*, 24, 1962.

[43] D. Werner. *Funktionalanalysis*. Springer, 2011.

[44] K. Königsberger. *Analysis 1*. Springer, 2004.

[45] M. Takesaki. *Theory of Operator Algebras I*. Springer, 1979.

[46] K. Berndl. *Zur Existenz der Dynamik in Bohmschen Systemen*. PhD thesis, 1994.

[47] K. Berndl, D. Dürr, S. Goldstein, G. Peruzzi and N. Zanghí. On the Global Existence of Bohmian Mechanics. *Communications in Mathematical Physics*, 173, 1995.

[48] W. Hunziker. On the Space-Time Behavior of Schrödinger Wavefunctions. *Journal of Mathematical Physics*, 7(2), 1966.

[49] T. Ozawa. Invariant subspaces for the Schrödinger evolution group. *Annales de l'Institut Henri Poincaré, Section A*, 54(1), 1991.

[50] K. Yajima. Existence of Solutions for Schrödinger Evolution Equations. *Communications in Mathematical Physics*, 110, 1987.

[51] T. Ozawa. Space-Time Behavior of Propagators for Schrödinger Evolution Equations with Stark Effect. *Journal of Functional Analysis*, 97, 1991.

[52] S. T. Kuroda and H. Morita. An estimate for solutions of Schrödinger equations with time-dependent potentials and associated scattering theory. *Journal of the Faculty of Science Univ. of Tokyo Section 1A Mathematics*, 24, 1977.

[53] F. A. Berezin and M. A. Shubin. *The Schrödinger Equation*. Springer, 1991.

[54] E. Zeidler. *Applied Functional Analysis – Applications to Mathematical Physics*. Springer, 1995.

[55] K. Königsberger. *Analysis 2*. Springer, 2000.