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Error analysis of tailor-made time integration schemes for certain classes of wave-type equations

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Abstract

This thesis is concerned with the time integration of three classes of wave-type partial differential equations. Each of these equations has numerical challenges, including nonlocal-in-time material laws, nontrivial boundary conditions, and an unbounded spatial domain. We construct tailor-made schemes and provide a rigorous numerical analysis.

We consider the semiclassical magnetic Schrödinger equation on the full space $\mathbb{R}^d$ with possibly time-dependent magnetic and electric potentials. For the approximation we use an appropriate Gaussian ansatz function, which leads to a set of ordinary differential equations. We show that in a special case, this ansatz function is the exact solution to the magnetic Schrödinger equation. Furthermore, we provide error bounds with respect to the semiclassical parameter in L^2-norm and we improve the error bound for relevant physical quantities of interest.

The second setting is concerned with a scattering problem for Maxwell's equations on an unbounded domain. The scatterer consists of a nonlocal-in-time material, which is modeled as a convolution in Maxwell's equations. In this situation, we use a coupling on the scatterer's bounded interface and derive a boundary integral equation. For the discretization we employ a convolution quadrature combined with a boundary element method. Finally, we show that this numerical approach is stable and we prove convergence rates.

For a semilinear viscoacoustic wave equation with a retarded material law and kinetic boundary conditions, we construct and analyze an implicit-explicit (IMEX) scheme. The IMEX scheme is computationally efficient, since it avoids the solution of nonlinear systems. The material law is described by a convolution term with exponential kernels. After applying an appropriate shift, we couple the convolution term as an auxiliary variable to the first-order system of partial differential equations. For the kinetic boundary conditions we make use of suitable bulk-surface Sobolev spaces to show wellposedness.

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CHAPTER 1

Introduction

The rich world of wave propagation appears in all kind of areas in everyday life, in scientific experiments, as well as in nature. Waves are the solution to a certain type of partial differential equations (PDEs). Thus, PDEs are a prolific tool for modeling the behavior of various scientific phenomena, which makes the understanding of wave-type PDEs valuable.

In quantum mechanics, the states of particles are described by wave functions, which depend on the particles position and time, cf. [58]. The most well-known application here is the propagation of light in free space, without any obstacles. However, in most applications we are interested in the interaction between waves and materials that have certain physical properties. This makes the wave-type PDE much more involved.

In geology, waves are used to discover the composition of the earth's surface by measuring the interaction of waves with the earth's different layers. The two main components of materials are a spring, i.e., elastic material, and a dashpot, which leads to a damping of the wave, cf. [101].

In optics, Maxwell's equations can be used to model the propagation of electromagnetic light waves and to investigate the influence of metamaterials on the waves. Possible observations include reflection, diffraction and absorption, cf. [37, 105].

However, the solution to a wave-type PDE is often not given analytically, which leads to the interest in approximating the solution to a PDE and the observation of its behavior over time. Numerical simulations of wave phenomena are desirable, e.g., in order to provide forecasts, or if experiments cannot be executed at the current situation. There are two major ideas to compute the numerical simulation. While space-time methods discretize time and space simultaneously in a common domain, we choose to separate time and space discretization. One advantage thereof is the possibility to use well-established solvers or tailor-made methods for either the space or time discretization.

One of the oldest numerical schemes is the method of lines, cf. [65], which leaves the time variable continuous and discretizes in space. The idea is to first perform a space discretization, which transforms the PDE into a system of ordinary differential equations that only depends on time and then apply a

time discretization.

If we decide to discretize in time first, also known as Rothe's method, cf. [39], we obtain a sequence of stationary PDEs to be solved in each time step. An advantage of Rothe's method is the possibility to adapt the space discretization in each time step according to the properties of the resulting stationary PDEs. This is particularly practicable for problems, where the solution changes its spatial support.

This thesis focuses on time integration of PDEs. We distinguish between implicit and explicit methods. In general, an implicit scheme takes the current approximated variable and solves a system of possibly nonlinear equations. However, after employing a space discretization, if nonlinear systems need to be solved, this may leads to prohibitively high computational costs.

In contrast, an explicit scheme calculates the next step by using only previously calculated approximations. However, in certain numerical experiments with explicit schemes, unexpected behavior of the approximation has been observed, cf. [64, Chap. 1]. This includes, e.g., very small stepsizes in order to obtain the desired accuracy even for problems that provide a smooth solution. This is caused by the fact that the stepsize is not determined by accuracy, but by stability. An example is the setting of chemical reactions, when fast reactions as well as slow reactions take place at the same time. We call a problem a stiff problem, if the approximation with an explicit scheme does not work, e.g., it will lead to an immense stepsize restriction in time or it produces oscillations, even though the exact solution does not oscillate. In this case, implicit schemes have lead to better results.

Each application we intend to simulate comes with its specialties and numerical difficulties. In this thesis, the following challenges arise.

- *The spatial domain*, on which the wave equation is posed, can be unbounded. Then, the space discretization with standard methods requires a truncation of the domain, such that nontrivial boundary conditions have to be imposed. Moreover, some applications require a high dimension of the domain, which leads to huge systems to be solved and high computational costs. This is also known as the curse of dimension. Our aim is to minimize this computational effort by providing more enhanced approximation techniques.

- *A convolution term* can model a certain type of materials. Since a standard time discretization of a convolution requires to store the discrete solution at all times, it produces a high memory cost.

- *Nontrivial boundary conditions* commonly appear in wave propagation. However, they are not covered by standard numerical analysis techniques and make the analysis much more involved. It is crucial to couple the dynamics on the boundary to the equation in such a way, that the resulting problem is well-posed. Furthermore, to ensure that the solution fulfills the boundary conditions, suitable function and discretization spaces need to be chosen. For the numerical discretization, a stable coupling of the wave equations on the boundary and the domain is required.

- *Nonlinearities* not only create analytical difficulties regarding wellposedness, a nonlinearity also has a major effect on the computational effort of a numerical method. This is due to the fact that a nonlinear inhomogeneity usually leads to solving a nonlinear system in each step of the time discretization.

- *Oscillations* in space of the exact solution to a wave-type equation, are difficult to approximate with standard mesh-based discretization methods. This is due to the fact, that we would have to use a very fine mesh, in order to obtain a reasonable approximation. However, this can lead to immense computational costs.

A priori knowledge of characteristics of solutions to wave-type equations can be used to find an appropriate method for simulating the behavior of the corresponding waves. It is our interest, to adjust a numerical method, such that it captures a certain quantity of interest, e.g., a physical property. However, the efficient implementation can be a challenging task.

In this thesis we consider three different settings of wave-type equations, where the numerical treatment is tailor-made for the respective property or challenge. The schemes are introduced and analyzed in two papers and one preprint, which are included in separate chapters. In Section 1.2, Section 1.3 and Section 1.4 we give short summaries of the main results for each topic.

The paper [31], included in Chapter 2, considers the approximation of the solution of a semiclassically scaled magnetic Schrödinger equation which describes the dynamics of charged particles under the influence of a magnetic field. The magnetic Schrödinger equation is posed in an unbounded domain. To tackle this difficult problem, we use an approximating manifold of complex Gaussians. A variational approach leads to ordinary differential equations for time-dependent parameters characterizing the approximating Gaussian. A novelty is, that we consider time-dependent electric and magnetic potentials.

If we intend to describe the magnetic potential by PDEs, we obtain Maxwell's equations. These are considered in Chapter 3, which contains the content of [113], accepted for publication in IMA Journal of Numerical Analysis. In this setting, the PDE is posed on an unbounded domain as well, but now we consider a scattering problem, where the wave travels through a bounded obstacle. Furthermore, the solution to Maxwell's equations fulfills a continuity requirement on the boundary. Here, we handle the challenge of approximating a wave on an unbounded domain by coupling the functions, inside and outside of the obstacle, on the boundary. Then, the space discretization is transferred to the boundary.

We emphasize, that the setting in Chapter 2 and Chapter 3 have in common, that the PDE is posed on an unbounded domain. In both cases, we use representation formulas. In Chapter 3 the exact solution can be described by a representation formula, which we then discretize. In contrast, in Chapter 2, we approximate by a representation formula. In both cases, the numerical approximations of the formulas lead to schemes that are numerically more favorable. The setting of Chapter 3 additionally contains a convolution, describing a nonlocal material, which is numerically treated by convolution quadrature.

Whereas the above mentioned papers deal with PDEs on an unbounded domain, in the preprint [32] included in Chapter 4, we consider the wave equation on a bounded domain with a smooth boundary. As in Chapter 3, the wave equation has a convolution term, which describes a nonlocal-in-time material law and a nontrivial boundary condition. In contrast to the scattering setting in Chapter 3, we do not use convolution quadrature, because the convolution kernels admit an additional differential equation, which can be coupled to the PDE. Moreover, the difficulty of the action on the boundary is solved by using bulk-surface Sobolev spaces. Since the domain is bounded, it is not necessary to restrict the space discretization to the boundary, but can be done with isoparametric finite elements.

1.1 Notation

Throughout this thesis, we denote the partial derivative with respect to time by $\partial_t u = u' = u_t$ and similarly for higher-order time derivatives.

Let $\Omega \subset \mathbb{R}^d$. We denote by $C(\Omega)$ the space of continuous functions on Ω. Furthermore, for k-times continuously differentiable functions on Ω, we use the notation $C^k(\Omega)$, where $k \in \mathbb{N}$. For the classical Lebesgue spaces we use the notation $L^p(\Omega)$, where $p \geq 1$, and $\mathcal{S}(\mathbb{R}^d)$ for the Schwartz space of rapidly decreasing functions. For $f, g \in L^2(\Omega)$, we denote the $L^2(\Omega)$ scalar product by

$$\langle f, g \rangle = \langle f \,|\, g \rangle = \int_\Omega \overline{f(x)} g(x) \, \mathrm{d}x.$$

We also use the dot product of $v, w \in \mathbb{R}^d$ or $v, w \in \mathbb{C}^d$ as $v \cdot w \coloneqq v^T w = v_1 w_1 + \cdots + v_d w_d$.

Let $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}_0^d$ be a multi-index and $|\alpha| = \alpha_1 + \ldots + \alpha_d$. For a sufficiently often weakly differentiable function f we define $\partial^\alpha f = \partial_1^{\alpha_1} \cdots \partial_d^{\alpha_d} f$. Let $k \in \mathbb{N}_0$, the k-th order Sobolev space is given by

$$H^k(\Omega) = \{ f : \Omega \to \mathbb{C} \mid \partial^\alpha f \in L^2(\Omega), \ |\alpha| \leq k \}.$$

We equip $H^k(\Omega)$ with the scalar product

$$\big(f, g\big)_{H^k(\Omega)} = \sum_{|\alpha| \leq k} \int_\Omega \overline{\partial^\alpha f(x)} \, \partial^\alpha g(x) \, \mathrm{d}x.$$

The Sobolev space $H^k(\Omega)$ with this scalar product is a Hilbert space. The canonical norm on $H^k(\Omega)$ is given by

$$\|f\|^2_{H^k(\Omega)} = \big(f, f\big)_{H^k(\Omega)}.$$

Let $\Omega \subset \mathbb{R}^d$ be bounded with boundary $\Gamma = \partial\Omega$. We introduce the notation

$$L^2(\Omega, \Gamma) = H^0(\Omega, \Gamma) = L^2(\Omega) \times L^2(\Gamma)$$

and define the following bulk-surface Sobolev spaces,

$$H^k(\Omega, \Gamma) = \left\{ v \in H^k(\Omega) \,\middle|\, \gamma_D(v) \in H^k(\Gamma) \right\}, \quad k \geq 1,$$

of $H^k(\Omega)$-functions with $H^k(\Gamma)$-traces, where γ_D denotes the Dirichlet trace operator, cf. [82]. We further equip $H^k(\Omega, \Gamma)$ with a scalar product, which induces the norm

$$\|v\|^2_{H^k(\Omega,\Gamma)} = \|v\|^2_{H^k(\Omega)} + \|\gamma_D(v)\|^2_{H^k(\Gamma)}, \qquad k \geq 0.$$

According to [72, Cor. 6.7] we know that $H^1(\Omega, \Gamma)$ is dense in $L^2(\Omega, \Gamma)$ and $C^\infty(\overline{\Omega})$ is dense in $H^1(\Omega, \Gamma)$. Whenever necessary, we will make use of weighted spaces. That is, for a Hilbert V with scalar product $(\cdot, \cdot)_V$ we define the weighted Hilbert space $\big(V_\mu, \ (\cdot, \cdot)_{V_\mu}\big)$, for some $\mu > 0$, by V equipped with the weighted scalar product, i.e.,

$$(x, y)_{V_\mu} = \mu (x, y)_V \quad \text{for} \quad x, y \in V.$$

Let Γ be C^1-regular. For a function $v \in H^1(\Omega)$ and the outer unit normal vector $\boldsymbol{n}$, we define the surface gradient

$$\nabla_\Gamma v = (\partial_{j,\Gamma} v)_{j=1}^d = (I - \boldsymbol{n}\boldsymbol{n}^T) \nabla v$$

and the Laplace-Beltrami operator

$$\Delta_\Gamma v = \sum_{j=1}^{d} \partial_{j,\Gamma}^2 v. \tag{1.2}$$

Let X, Y be Banach spaces and $K : X \to Y$ a bounded linear operator. We define the operator norm

$$\|K\|_{Y \leftarrow X} = \max_{x \in X,\ \|x\|_X = 1} \|Kx\|_Y .$$

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with Lipschitz boundary $\Gamma = \partial\Omega$ or the complement of the closure of such a domain. Furthermore, let $\mathbf{v}$ be a vector field on Ω, and we employ the standard weak definition of the **curl** operator and denote the corresponding Sobolev space by

$$H(\mathbf{curl}, \Omega) = \{\mathbf{v} \in \boldsymbol{L}^2(\Omega) \,|\, \mathbf{curl}\, \mathbf{v} \in \boldsymbol{L}^2(\Omega)\}.$$

For a continuous vector field $\mathbf{v} : \overline{\Omega} \to \mathbb{C}^3$, we define the tangential trace

$$\gamma_T \mathbf{v} = \mathbf{v}|_\Gamma \times \boldsymbol{n} \qquad \text{on } \Gamma, \tag{1.3}$$

where $\boldsymbol{n}$ denotes the unit normal vector pointing into the exterior (unbounded) domain.

For continuous tangential vector fields on the boundary $\boldsymbol{\phi}, \psi : \Gamma \to \mathbb{C}^3$, we define a skew-hermitian sesquilinear form,

$$[\boldsymbol{\phi}, \psi]_\Gamma = \int_\Gamma (\boldsymbol{\phi} \times \boldsymbol{n}) \cdot \psi \, \mathrm{d}\sigma. \tag{1.4}$$

The trace can be extended to a surjective bounded linear operator $\gamma_T : H(\mathbf{curl}, \Omega) \to \gamma_T(H(\mathbf{curl}, \Omega))$, cf. [30] and [29, Sect. 2.2]. We define the trace space $\mathrm{X}_\Gamma = \gamma_T(H(\mathbf{curl}, \Omega))$, which is a Hilbert space.The pairing $[\cdot, \cdot]_\Gamma$ can be extended to a continuous sesquilinear form on $\mathrm{X}_\Gamma \times \mathrm{X}_\Gamma$, such that X_Γ is its own dual.

Let X be a Hilbert space. We denote by $H^r(\mathbb{R}, X)$ the Sobolev space of order r of X-valued functions on $\mathbb{R}$. On a finite interval $(0, T)$ we define

$$H_0^r(0, T; X) = \{g|_{(0,T)} \,|\, g \in H^r(\mathbb{R}, X) \ \text{ with } \ g = 0 \ \text{ on } \ (-\infty, 0)\}, \tag{1.5}$$

where the subscript 0 in H_0^r only indicates the vanishing condition for the left end-point of the interval.

Let $s \in \mathbb{C}$ with $\operatorname{Re} s > 0$ and let f be a possibly vector-valued function on the nonnegative real line. We denote Laplace transform by

$$\widehat{f}(s) = \mathcal{L}(f)(s) = \int_0^\infty f(t)\, \mathrm{e}^{-ts} \, \mathrm{d}t, \tag{1.6}$$

whenever it is well-defined. Provided that f is sufficiently regular, the Laplace transform $\widehat{f}$ is an analytic function on the right half plane $\{s \in \mathbb{C} \mid \operatorname{Re} s > 0\}$.

1.2 Results of Gaussians for the magnetic Schrödinger equation

The semiclassical magnetic Schrödinger equation describes the behavior of particles exposed to the force of an external magnetic vector potential A with $\operatorname{div} A = 0$. That is, we seek ψ, such that

$$\mathrm{i}\varepsilon\partial_t\psi(t) = H(t)\psi(t), \quad \psi(0) = \psi_0, \quad t \in \mathbb{R} \tag{1.7a}$$

on $\mathbb{R}^d$ with the magnetic Hamiltonian

$$H(t) = -\frac{\varepsilon^2}{2}\Delta + \mathrm{i}\varepsilon A(t)\cdot\nabla + \widetilde{V}(t), \qquad \widetilde{V}(t) = \frac{1}{2}|A(t)|^2 + V(t), \tag{1.7b}$$

initial value $\psi_0 \in L^2(\mathbb{R}^d)$, and with a semiclassical parameter $0 < \varepsilon \ll 1$. The scalar potential V acts as an electric potential. One can interpret the small semiclassical parameter as the mass ratio of light electrons and heavy nucleons which appear in a molecule.

For the numerical simulation, the magnetic Schrödinger equation is challenging for several reasons. First, it is posed on the full space $\mathbb{R}^d$, which means, one has to truncate the area of simulation. Second, the solution to the magnetic Schrödinger equation is highly oscillatory. In order to capture these oscillations, we would have to use a fine discretization. In realistic applications, where molecules are considered, we have a large number of electrons and protons, leading to a high-dimensional problem. Combined with the small stepsize, this leads to a huge computational effort, making the discretization with standard finite elements unfeasible.

To overcome this difficulty, in [98], Lubich suggests to take a manifold $\mathcal{M}$ of ansatz functions, which contains, under certain conditions, the exact solution to the Schödinger equation. These ansatz functions, which we also refer to as Gaussian wave packets, are localized Gaussians of the form

$$u(t,x) = \exp\Big(\frac{\mathrm{i}}{\varepsilon}\big(\frac{1}{2}(x-q(t))^T\mathcal{C}(t)(x-q(t)) + (x-q(t))^T p(t) + \zeta(t)\big)\Big),$$

where $q, p \in \mathbb{R}^d$ can be interpreted as position center and momentum, $\mathcal{C} \in \mathbb{C}^{d\times d}$ is the width matrix of the packet. The matrix $\mathcal{C}$ has a positive definite imaginary part, which characterizes the slope around the position. Finally, we have a phase and weight parameter $\zeta \in \mathbb{C}$. Numerically, the main advantage of the Gaussians is, that they are fully described by their time-dependent parameters $q, p, \mathcal{C}$, and ζ. For these parameters, we derive ordinary differential equations (ODEs) to approximate the solution to the magnetic Schrödinger equation.

Next, we sketch the approximation by a Gaussian wave packet. To this end, we mention that the set of Gaussian wave packets forms a manifold $\mathcal{M}$. The tangential space at $u(t)$ is denoted by $\mathcal{T}_{u(t)}\mathcal{M}$. The approximating Gaussian wave packet is characterized by the Dirac–Frenkel variational formulation, cf. [87, 98], i.e., seek $u(t) \in \mathcal{M}$ such that for all $t \in \mathbb{R}$ it holds

$$\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}, \quad \big\langle \mathrm{i}\varepsilon\partial_t u(t) - H(t)u(t) | v\big\rangle = 0 \quad \text{for all} \quad v \in \mathcal{T}_{u(t)}\mathcal{M},$$

with initial value $u(0) = u_0 \in \mathcal{M}$. Employing the orthogonal projection $P_u : L^2(\mathbb{R}^d) \to \mathcal{T}_u\mathcal{M}$ onto the tangent space, this can be reformulated to

$$\mathrm{i}\varepsilon\partial_t u(t) = P_{u(t)}\big(H(t)u(t)\big), \quad u(0) = u_0 \in \mathcal{M}. \tag{1.8}$$

It is crucial to use the composition of the tangent space. In this case, it is made up of Gaussians multiplied with a d-variate polynomial of degree at most two. The next key step is to properly investigate the projection onto the tangent space and observe that here, it can be reduced to a multiplication operator.

The approximation by Gaussian wave packets seems appropriate due to the following exactness result.

Proposition 1.1 ([87, Prop. 3.2]). *Let $V(t,\cdot)$ be quadratic and $A(t,\cdot)$ be linear in space for all $t \in \mathbb{R}$. If $\psi_0 \in \mathcal{M}$ is a Gaussian, then the variational approximation u defined by (1.8) is exact, i.e., $u(t) = \psi(t)$, where ψ denotes the solution of (1.7a).*

We measure the quality of the approximation by the Gaussian wave packets in the L^2-norm and using a physically motivated observable error bound, which will be given with respect to the semiclassical parameter ε. We derive these two error bounds provided that the following assumption is fulfilled.

Assumption 1.2. *The scalar potential $\widetilde{V}\colon \mathbb{R}\times\mathbb{R}^d \to \mathbb{R}$ and the vector valued potential $A = (A_j)_{j=1,\dots,d}\colon \mathbb{R}\times\mathbb{R}^d \to \mathbb{R}^d$ are infinitely often differentiable and in addition*

(a) *$\widetilde{V}$ is subquadratic, i.e., $\nabla^k \widetilde{V}$ is bounded for all $k \geq 2$, and*

(b) *A is sublinear, i.e., $\nabla^k A$ is bounded for all $k \geq 1$, and satisfies $\operatorname{div} A = 0$.*

The following error estimate extends the well-known error bound, e.g., [87], to the magnetic case.

Theorem 1.3. *Let ψ, u be the solution of (1.7a) and (1.8), respectively, and let $\psi_0 = u_0 \in \mathcal{M}$ be L^2-normalized Gaussians. Then, the error bound*

$$\|\psi(t) - u(t)\|_{L^2} \leq tc\sqrt{\varepsilon}, \qquad t \in [0,T],$$

holds with a constant c which depends on the parameters' growth for the time-interval $[0,T]$, in particular on the width matrix $\mathcal{C}$, and on the potentials, but is independent of ε and t.

In classical mechanics, at a time $t \in \mathbb{R}$, a single particle is characterized by its position and momentum variables $\widetilde{q}(t), \widetilde{p}(t) \in \mathbb{R}^3$, [98, Chapt 1]. The setting is readily extended to the case of multiple particles. Then, a potential V acting on the position variables of N particles describes their interaction and the total kinetic energy T is given as the sum of kinetic energies,

$$V(\widetilde{q}) = V(\widetilde{q}_1, \dots, \widetilde{q}_N) \qquad \text{and} \qquad T(\widetilde{p}) = \frac{1}{2}\sum_{j=1}^{N} |\widetilde{p}_j|^2 .$$

This can be generalized to smooth functions $\boldsymbol{a} = \boldsymbol{a}(\widetilde{q},\widetilde{p}) \in C^\infty(\mathbb{R}^{2d})$, where $d = 3N$, acting on the position and momentum variables. We call them classical observables. The classical equations of motion for charged particles in a magnetic field are given by the Hamilton system, which is induced by the time-dependent Hamiltonian function, cf. [58, 67],

$$h(t,\widetilde{q},\widetilde{p}) = \frac{1}{2}|\widetilde{p}|^2 - A(t,\widetilde{q})\cdot\widetilde{p} + \widetilde{V}(t,\widetilde{q}), \quad (t,\widetilde{q},\widetilde{p}) \in \mathbb{R}\times\mathbb{R}^{2d}. \tag{1.9}$$

The Hamilton system then reads

$$\begin{aligned} \dot{\widetilde{q}}(t) &= \widetilde{p}(t) - A(t,\widetilde{q}(t)), & \widetilde{q}(0) &= \widetilde{q}_0, \\ \dot{\widetilde{p}}(t) &= J_A^T(t,\widetilde{q}(t))\widetilde{p}(t) - \nabla\widetilde{V}(t,\widetilde{q}(t)), & \widetilde{p}(0) &= \widetilde{p}_0, \end{aligned} \tag{1.10}$$

where J_A denotes the Jacobian matrix with respect to the spatial variable of A. Employing standard ODE theory, we see that (1.10) admits a global solution. This gives rise to the classical propagator

$$\Phi^{t,s} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}, \quad (\widetilde{q}(s),\widetilde{p}(s)) \mapsto (\widetilde{q}_s(t),\widetilde{p}_s(t)),$$

that maps initial values at time s to the solution of (1.10) at time t.

In the quantum mechanic case, the current state of N particles is characterized by a wave function $\psi : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C}$ with $d = 3N$. For every classical observable $\boldsymbol{a} \in C^\infty(\mathbb{R}^{2d})$, we associate a quantum observable $\mathbf{A} = \mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})$ via the Weyl quantization, i.e., formally, for a Schwartz function $\varphi \in \mathcal{S}(\mathbb{R}^d)$, we define

$$\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})\varphi(x) \coloneqq \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^{2d}} \boldsymbol{a}\Big(\frac{x+\widetilde{q}}{2}, \widetilde{p}\Big) \mathrm{e}^{\mathrm{i}\widetilde{p}\cdot(x-\widetilde{q})/\varepsilon} \varphi(\widetilde{q})\, \mathrm{d}(\widetilde{q}, \widetilde{p}) \qquad x \in \mathbb{R}^d.$$

It has the property that

$$\mathrm{op}_{\mathrm{Weyl}}(\widetilde{q})\varphi = -\mathrm{i}\varepsilon\nabla\psi, \qquad \text{and} \qquad \mathrm{op}_{\mathrm{Weyl}}(\widetilde{p})\varphi = x\varphi,$$

and for the energy we have

$$\mathrm{op}_{\mathrm{Weyl}}(h(t, \widetilde{q}, \widetilde{p}))\varphi = H(t)\varphi$$

with the classical Hamiltonian function (1.9). The propagation of the observable along the solution to the Schrödinger equation (1.7a) is of physical interest. It is defined by averages $\langle \mathbf{A} \rangle_\psi$ with respect to the L^2-scalar product, i.e.,

$$\langle \mathbf{A} \rangle_\psi = \langle \psi | \mathbf{A}\psi \rangle = \int_{\mathbb{R}^d} \overline{\psi(x)} (\mathbf{A}\psi)(x)\, \mathrm{d}x.$$

For a certain class of quantum observables we compare their propagation along the exact and variational solution, and show an improved semiclassical error bound. For the proof it is crucial to relate quantum observables and classically propagated observables, which results in a time-dependent version of Egorov's theorem, that is proven in Chapter 2. The version of Egorov's theorem, which is well-established in semiclassical analysis, is only provided for a time-independent setting.

Theorem 1.4. *Let ψ, u be the solution of (1.7a) and (1.8), respectively, and let $\psi_0 = u_0 \in \mathcal{M}$ be L^2-normalized Gaussians. Moreover, let $\mathbf{A} = \mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})$ be a quantum observable stemming from a classical observable, such that $\boldsymbol{a}$ and the composition with the classical flow $\boldsymbol{a} \circ \Phi^{t,s}$ have bounded derivatives of order ≥ 1. Then we have the error bound*

$$\big| \langle \psi(t) | \mathbf{A}\psi(t) \rangle - \langle u(t) | \mathbf{A}u(t) \rangle \big| \leq t\, c\, \varepsilon^2$$

for all $t \in [0, T]$. The error constant c depends on the parameters' growth for the time-interval $[0, T]$, in particular on the width matrix $\mathcal{C}$, on the potentials A, $\widetilde{V}$, and on $\boldsymbol{a}$, but is independent of ε and t.

The initial idea to investigate the problem (1.7a) relies on the results in the review article by Lasser and Lubich, where Gaussian approximations and their corresponding ODEs are known for the case $A = 0$ and time-independent, electric potential $\widetilde{V}$. There, Lasser and Lubich introduce a new observable error bound of order $\mathcal{O}(\varepsilon)$. This error bound was improved by Ohsawa to the order $\mathcal{O}(\varepsilon^{3/2})$. Our contribution, which is given in Chapter 2 and published in [31], relies in extending the results to the magnetic case and including time-dependent electric and magnetic potentials. Furthermore, in [31], we generalize to the case, where the Hamilton operator in the Schrödinger equation (1.7a) is generated by a smooth, classical Hamiltonian function, which has bounded derivatives of order ≥ 2. Finally, we were able to improve the observable error bound to the order $\mathcal{O}(\varepsilon^2)$.

Outlook The idea of approximation by Gaussian wave packets can be extended to the approximation by an element made up of an orthonormal basis of Gaussians with a polynomial prefactor. These are called the Hagedorn wave packets. This has been done in, e.g., [59–61] and [87, Sec. 4] for the non-magnetic case. Hagedorn wave packets for the magnetic Schrödinger equation with a linear magnetic potential are considered in [56, 57]. We are confident, that the results shown in [31] can also be shown for Hagedorn wave packets. Possibly, higher-order approximations in terms of the semiclassical parameter ε can be achieved. The authors of the preprint [79] consider an approach with a mixture of time-dependent Hagedorn wave packets and time-independent basis functions.

A new representation of square-integrable function by a superposition of Gaussian wave packets is analyzed in [20]. Our results are the basis for the paper [124], dealing with the efficient implementation of the parameters' ODEs by Boris algorithm. For a more detailed literature review, see the references in [31].

1.3 Results of time-dependent electromagnetic scattering from dispersive materials

We consider the propagation of electromagnetic waves on a possibly unbounded domain $\Omega \subset \mathbb{R}^3$. In this setting, we assume vanishing current and charge. Then the situation can be modeled by the time-dependent Maxwell's equations. That is, we seek $\boldsymbol{E}$ and $\boldsymbol{H}$, such that

$$\begin{aligned} \varepsilon_0(\partial_t \boldsymbol{E} + \boldsymbol{P}(\partial_t \boldsymbol{E})) - \mathbf{curl}\, \boldsymbol{H} &= 0, \\ \mu_0(\partial_t \boldsymbol{H} + \boldsymbol{M}(\partial_t \boldsymbol{H})) + \mathbf{curl}\, \boldsymbol{E} &= 0, \end{aligned} \qquad \text{in } \Omega,$$

where ε_0 and μ_0 denote the constant permittivity and permeability, respectively, and the polarization field $\boldsymbol{P}$ and the magnetization field $\boldsymbol{M}$ are given by a convolution in time

$$\boldsymbol{P}(\boldsymbol{E})(t) = \int_0^t \chi_e(\theta)\boldsymbol{E}(t-\theta)\,\mathrm{d}\theta, \qquad \boldsymbol{M}(\boldsymbol{H})(t) = \int_0^t \chi_m(\theta)\boldsymbol{H}(t-\theta)\,\mathrm{d}\theta,$$

with scalar susceptibility kernels χ_e and χ_m. These are characterized by physical properties of the material. In the case of vanishing susceptibility kernels, this model describes the situation of vacuum. Common metamaterials that fit into this framework are provided by the Drude or Lorentz model. The Lorentz oscillators, for example, use the susceptibility kernels with $\ell \in \{e, m\}$

$$\chi_\ell(t) = \frac{\beta_\ell}{\lambda_\ell} \mathrm{e}^{-\frac{\alpha_\ell}{2}t} \sin(\lambda_\ell t), \qquad \lambda_\ell = \sqrt{\omega_\ell^2 - \frac{\alpha_\ell}{4}}, \tag{1.11}$$

where ω_ℓ is the resonance frequency, $0 < \alpha_\ell < 4\omega_\ell^2$ is a damping coefficient and $\beta_\ell > 0$ gives the strength. For more information, we refer to the survey [37].

The physical properties of the material are usually obtained from experiments in the frequency domain, i.e., the susceptibility kernels are given as a transfer function with respect to a frequency variable $s \in \mathbb{C}$ as opposed to a time-dependent function. Employing the Laplace transforms $(\widehat{\chi}_e^{\pm}(s), \widehat{\chi}_m^{\pm}(s))$ of the susceptibility kernels $(\chi_e^{\pm}(t), \chi_m^{\pm}(t))$, cf. (1.6), we define the time-harmonic kernels

$$\varepsilon^{\pm}(s) = \varepsilon_0(1 + \widehat{\chi}_e^{\pm}(s)), \qquad \mu^{\pm}(s) = \mu_0(1 + \widehat{\chi}_m^{\pm}(s)). \tag{1.12}$$

Without providing further details, let us note, that the time-harmonic kernels are bounded and fulfill a strong passivity condition. This has physical applications, as explained in [37, after Definition 2.5].

From now on, we consider an incoming electromagnetic wave $(\boldsymbol{E}_{\mathrm{inc}}, \boldsymbol{H}_{\mathrm{inc}})$ that travels in $\mathbb{R}^3$ and hits a bounded scatterer $\Omega^- \subset \mathbb{R}^3$, which we refer to as the interior domain. Furthermore, we assume, that at the beginning of the observation, the incoming wave is away from the scatterer, leading to vanishing initial conditions at the boundary. When the incoming electromagnetic wave reaches Ω^-, the scatterer interacts with the wave, e.g., by reflection, and travels on as a scattered wave. We distinguish between the scattered wave $(\boldsymbol{E}^+, \boldsymbol{H}^+)$ in the exterior domain Ω^+ and the scattered wave $(\boldsymbol{E}^-, \boldsymbol{H}^-)$ inside of the scatterer. In the present situation, the scatterer consists of a nonlocal material, i.e., an interaction with the wave has a non-instantaneous effect on the scatterer. More precisely, any prior interaction with the scatterer also has an impact on the scattered wave at later times. The scattering problem reads

$$\begin{aligned} \varepsilon_0(\partial_t \boldsymbol{E}^- + \boldsymbol{P}(\partial_t \boldsymbol{E}^-)) - \mathbf{curl}\, \boldsymbol{H}^- &= 0, \\ \mu_0(\partial_t \boldsymbol{H}^- + \boldsymbol{M}(\partial_t \boldsymbol{H}^-)) + \mathbf{curl}\, \boldsymbol{E}^- &= 0, \end{aligned} \qquad \text{in the interior domain } \Omega^-, \tag{1.13a}$$

and

$$\begin{aligned} \varepsilon_0 \partial_t \boldsymbol{E}^+ - \mathbf{curl}\, \boldsymbol{H}^+ &= 0, \\ \mu_0 \partial_t \boldsymbol{H}^+ + \mathbf{curl}\, \boldsymbol{E}^+ &= 0, \end{aligned} \qquad \text{in the exterior domain} \quad \Omega^+. \tag{1.13b}$$

Furthermore, the electromagnetic waves behave continuously along the interface of the scatterer $\Gamma = \partial\Omega^{\pm}$. Thus, we enforce transmission conditions

$$\begin{aligned} \gamma_T \boldsymbol{E}^- &= \gamma_T \boldsymbol{E}^+ + \gamma_T \boldsymbol{E}_{\text{inc}}, \\ \gamma_T \boldsymbol{H}^- &= \gamma_T \boldsymbol{H}^+ + \gamma_T \boldsymbol{H}_{\text{inc}}, \end{aligned} \qquad \text{on } \Gamma,$$

with the tangential trace γ_T, defined in (1.3).

Numerically, the scattering problem (1.13) has two main challenges. First, the nonlocal-in-time behavior of the convolution term demands for a standard time discretization method to store a complete history of the solution. Second, the exterior domain Ω^+ is unbounded, making a standard space discretization impractical, since the domain will then need a truncation.

To overcome these difficulties, we use the following techniques. Our focus lies on the traces of the electromagnetic waves on the scatterer's bounded interface Γ and we derive a time-harmonic boundary integral equation (BIE). This BIE maps the given boundary traces of the external incoming waves to the traces of the scattered exterior and interior fields, respectively. Then, we employ a representation formula based on the fundamental solutions to Maxwell's equations. This formula only uses the information on the boundary and restores the electromagnetic fields $(\boldsymbol{E}^{\pm}, \boldsymbol{H}^{\pm})$ in the outer and inner domain. We show wellposedness of the time-harmonic BIE by applying a Lax-Milgram theorem. Finally, we employ a Runge-Kutta based convolution quadrature for the time discretization.

Time-harmonic scattering and transmission problem As mentioned before, in applications we typically are given a transfer function with respect to a frequency variable $s \in \mathbb{C}$. To relate functions on the frequency domain to the time domain we employ the Heaviside notation. That is, let $\boldsymbol{g} : [0, \infty) \to \mathbb{R}$ be sufficiently regular and extended by 0 for $t < 0$ and let ε be an analytic function for $\operatorname{Re} s > 0$. Then, we associate to ε a time-dependent convolution

$$\varepsilon(\partial_t)\boldsymbol{g}(t) = \int_0^\infty (\mathcal{L}^{-1}\varepsilon)(\theta)\, \boldsymbol{g}(t-\theta)\, \mathrm{d}\theta, \qquad t > 0, \tag{1.14}$$

with the differential calculus ∂_t and the inverse Laplace transform $\mathcal{L}^{-1}$. For example, the function $\varepsilon(s) = s$ corresponds to the time derivative ∂_t in the time domain, provided g has vanishing initial conditions. Moreover, it is well known that the Laplace transform of a convolution translates into a multiplication of the Laplace transformed convolution kernels. The previous considerations give rise to applying the Laplace transform to the scattering problem (1.13). We denote the Laplace transformed electromagnetic fields by $\widehat{\boldsymbol{E}} = \mathcal{L}(\boldsymbol{E})$, cf. (1.6). Then, with the time-harmonic kernels (1.12), the time-harmonic scattering problem reads

$$\begin{aligned} \varepsilon^{\pm}(s) s \widehat{\boldsymbol{E}}^{\pm} - \mathbf{curl}\, \widehat{\boldsymbol{H}}^{\pm} &= 0 \\ \mu^{\pm}(s) s \widehat{\boldsymbol{H}}^{\pm} + \mathbf{curl}\, \widehat{\boldsymbol{E}}^{\pm} &= 0 \end{aligned} \qquad \text{in } \Omega^{\pm},$$

with the transmission conditions

$$\begin{aligned} \gamma_T \widehat{\boldsymbol{E}}^+ + \gamma_T \widehat{\boldsymbol{E}}^+_{\text{inc}} &= \gamma_T \widehat{\boldsymbol{E}}^- \\ \gamma_T \widehat{\boldsymbol{H}}^+ + \gamma_T \widehat{\boldsymbol{H}}^+_{\text{inc}} &= \gamma_T \widehat{\boldsymbol{H}}^- \end{aligned} \qquad \text{on } \Gamma. \tag{1.15a}$$

To state the representation formula, which enables us to handle the unbounded domain, we reformulate the time-harmonic scattering problem (1.15) into an electromagnetic transmission problem on $\mathbb{R}^3 \setminus \Gamma$. The transmission problem includes jumps and averages for the tangential traces defined by

$$[\gamma_T] = \gamma_T^+ - \gamma_T^-, \qquad \{\gamma_T\} = \tfrac{1}{2}\left(\gamma_T^+ + \gamma_T^-\right).$$

Before stating the transmission problem, let us point out the following important observation. If the electromagnetic wave $(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{H}})$ on $\mathbb{R}^3 \setminus \Gamma$ solves the time-harmonic transmission problem, then the restrictions $\widehat{\boldsymbol{E}}^{\pm} = \widehat{\boldsymbol{E}}|_{\Omega^{\pm}}$ and $\widehat{\boldsymbol{H}}^{\pm} = \widehat{\boldsymbol{H}}|_{\Omega^{\pm}}$ solve the time-harmonic scattering problem (1.15) with boundary densities $(\widehat{\boldsymbol{\varphi}}, \widehat{\psi}) = (-\gamma_T \widehat{\boldsymbol{H}}^+_{\mathrm{inc}}, \gamma_T \widehat{\boldsymbol{E}}^+_{\mathrm{inc}})$.

Let $(\widehat{\boldsymbol{\varphi}}, \widehat{\psi})$ be sufficiently regular boundary densities. The time-harmonic transmission problem reads

$$\varepsilon(s) s \widehat{\boldsymbol{E}} - \mathbf{curl}\, \widehat{\boldsymbol{H}} = 0 \qquad \text{in} \quad \mathbb{R}^3 \setminus \Gamma, \tag{1.16a}$$

$$\mu(s) s \widehat{\boldsymbol{H}} + \mathbf{curl}\, \widehat{\boldsymbol{E}} = 0 \qquad \text{in} \quad \mathbb{R}^3 \setminus \Gamma, \tag{1.16b}$$

$$[\gamma_T] \widehat{\boldsymbol{H}} = \widehat{\boldsymbol{\varphi}}, \tag{1.16c}$$

$$-[\gamma_T] \widehat{\boldsymbol{E}} = \widehat{\psi}. \tag{1.16d}$$

It is solved by the electromagnetic fields $(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{H}})$ given by

$$\widehat{\boldsymbol{E}} = -\frac{\sqrt{\mu(s)}}{\sqrt{\varepsilon(s)}} \boldsymbol{\mathcal{S}}_{\varepsilon,\mu}(s) \widehat{\boldsymbol{\varphi}} + \boldsymbol{\mathcal{D}}_{\varepsilon,\mu}(s) \widehat{\psi}, \qquad \widehat{\boldsymbol{H}} = -\boldsymbol{\mathcal{D}}_{\varepsilon,\mu}(s) \widehat{\boldsymbol{\varphi}} - \frac{\sqrt{\varepsilon(s)}}{\sqrt{\mu(s)}} \boldsymbol{\mathcal{S}}_{\varepsilon,\mu}(s)\, \widehat{\psi}, \tag{1.17}$$

where $\boldsymbol{\mathcal{S}}_{\varepsilon,\mu}(s)$, $\boldsymbol{\mathcal{D}}_{\varepsilon,\mu}(s)$ are potential operators, based on the fundamental solution of the time-harmonic Maxwell's equations. We will not go into detail here and refer to [29, 106] for further information. The identities in (1.17) are representation formulas for the solutions $\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{H}}$, which can be derived from known *jump relations*, cf. [29, 106]. We emphasize that the representation formulas map boundary densities to electromagnetic fields on the inner and the outer domain.

Boundary integral equation and representation We now turn towards the derivation of the BIE. To this end, the Calderón operator plays an important role by linking the interior and exterior domain. For $s \in \mathbb{C}$ with $\operatorname{Re} s > 0$ the Calderón operator $\boldsymbol{C}_{\varepsilon,\mu}(s) : \mathrm{X}_\Gamma^2 \to \mathrm{X}_\Gamma^2$ is constructed, cf. [85], such that it maps jumps of the solution $(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{H}})$ to (1.16) to their averages,

$$\boldsymbol{C}_{\varepsilon,\mu}(s) \begin{pmatrix} [\gamma_T]\widehat{\boldsymbol{H}} \\ -[\gamma_T]\widehat{\boldsymbol{E}} \end{pmatrix} = \begin{pmatrix} \{\gamma_T\}\widehat{\boldsymbol{E}} \\ \{\gamma_T\}\widehat{\boldsymbol{H}} \end{pmatrix}. \tag{1.18}$$

Crucial properties of the Calderón operator are boundedness and coercivity. For the coercivity, we note that the skew-hermitian pairing $[\cdot,\cdot]_\Gamma$ defined in (1.4) is extended from $\mathrm{X}_\Gamma \times \mathrm{X}_\Gamma$ to $\mathrm{X}_\Gamma^2 \times \mathrm{X}_\Gamma^2$ in the natural way,

$$\left[\begin{pmatrix} \boldsymbol{\varphi} \\ \psi \end{pmatrix}, \begin{pmatrix} \boldsymbol{\upsilon} \\ \boldsymbol{\xi} \end{pmatrix} \right]_\Gamma = [\boldsymbol{\varphi}, \boldsymbol{\upsilon}]_\Gamma + [\psi, \boldsymbol{\xi}]_\Gamma.$$

The family of linear operators is of positive type, i.e., for $\operatorname{Re} s > 0$ and all $(\boldsymbol{\varphi}, \psi) \in \mathrm{X}_\Gamma^2$, we have

$$\operatorname{Re} \left[\begin{pmatrix} \boldsymbol{\varphi} \\ \psi \end{pmatrix}, \boldsymbol{C}_{\varepsilon,\mu}(s) \begin{pmatrix} \boldsymbol{\varphi} \\ \psi \end{pmatrix} \right]_\Gamma \geq C(\varepsilon, \mu, \Gamma) \frac{\operatorname{Re} s}{|s|^2 + 1} \left(\|\boldsymbol{\varphi}\|^2_{\mathrm{X}_\Gamma} + \|\psi\|^2_{\mathrm{X}_\Gamma} \right), \tag{1.19}$$

where the constant $C(\varepsilon,\mu,\Gamma)$ depends on bounds of the physical functions ε, μ and the boundary Γ. Furthermore, it satisfies the bound

$$\|\boldsymbol{C}_{\varepsilon,\mu}(s)\|_{\mathrm{X}_\Gamma^2\leftarrow\mathrm{X}_\Gamma^2}\leq C(\varepsilon,\mu,\Gamma)\,\frac{|s|^2+1}{\operatorname{Re} s}, \tag{1.20}$$

where $C(\varepsilon,\mu,\Gamma)$ depends on bounds of the physical functions ε, μ and the boundary Γ. To derive the BIE, we introduce the notation

$$\widehat{\boldsymbol{\phi}}^+=\begin{pmatrix}\widehat{\boldsymbol{\varphi}}^+\\ \widehat{\boldsymbol{\psi}}^+\end{pmatrix}=\begin{pmatrix}\gamma_T^+\widehat{\boldsymbol{H}}^+\\ -\gamma_T^+\widehat{\boldsymbol{E}}^+\end{pmatrix},\qquad \widehat{\boldsymbol{\phi}}^-=\begin{pmatrix}\widehat{\boldsymbol{\varphi}}^-\\ \widehat{\boldsymbol{\psi}}^-\end{pmatrix}=\begin{pmatrix}-\gamma_T^-\widehat{\boldsymbol{H}}^-\\ \gamma_T^-\widehat{\boldsymbol{E}}^-\end{pmatrix},\qquad \widehat{\boldsymbol{g}}^{\mathrm{inc}}=\frac{1}{2}\begin{pmatrix}\gamma_T^+\widehat{\boldsymbol{E}}^+_{\mathrm{inc}}\\ \gamma_T^+\widehat{\boldsymbol{H}}^+_{\mathrm{inc}}\end{pmatrix}. \tag{1.21}$$

Further, we use relation (1.18) and the transmission conditions (1.15a), which yield

$$\boldsymbol{C}_{\varepsilon^+,\mu^+}(s)\widehat{\boldsymbol{\phi}}^+=-\boldsymbol{J}\widehat{\boldsymbol{\phi}}^--\widehat{\boldsymbol{g}}^{\mathrm{inc}}\quad\text{and}\quad\boldsymbol{C}_{\varepsilon^-,\mu^-}(s)\widehat{\boldsymbol{\phi}}^-=\boldsymbol{J}\widehat{\boldsymbol{\phi}}^++\widehat{\boldsymbol{g}}^{\mathrm{inc}}$$

with an appropriate block operator $\boldsymbol{J}$. This is collected in the time-harmonic BIE

$$\boldsymbol{A}(s)\begin{pmatrix}\widehat{\boldsymbol{\phi}}^+\\ \widehat{\boldsymbol{\phi}}^-\end{pmatrix}=\begin{pmatrix}-\widehat{\boldsymbol{g}}^{\mathrm{inc}}\\ \widehat{\boldsymbol{g}}^{\mathrm{inc}}\end{pmatrix},\quad\text{where}\quad\boldsymbol{A}(s)=\begin{pmatrix}\boldsymbol{C}_{\varepsilon^+,\mu^+}(s) & \boldsymbol{J}\\ -\boldsymbol{J} & \boldsymbol{C}_{\varepsilon^-,\mu^-}(s)\end{pmatrix}:\mathrm{X}_\Gamma^4\to\mathrm{X}_\Gamma^4. \tag{1.22}$$

This BIE is considered in its weak formulation. For $\operatorname{Re} s>0$ and given $\widehat{\boldsymbol{g}}^{\mathrm{inc}}\in\mathrm{X}_\Gamma^2$, find $(\boldsymbol{\phi}^+,\boldsymbol{\phi}^-)\in\mathrm{X}_\Gamma^4$ such that, for all $(\boldsymbol{\upsilon},\boldsymbol{\xi})\in\mathrm{X}_\Gamma^4$

$$\left[\begin{pmatrix}\boldsymbol{\upsilon}\\ \boldsymbol{\xi}\end{pmatrix},\boldsymbol{A}(s)\begin{pmatrix}\boldsymbol{\phi}^+\\ \boldsymbol{\phi}^-\end{pmatrix}\right]_\Gamma=\left[\begin{pmatrix}\boldsymbol{\upsilon}\\ \boldsymbol{\xi}\end{pmatrix},\begin{pmatrix}-\widehat{\boldsymbol{g}}^{\mathrm{inc}}\\ \widehat{\boldsymbol{g}}^{\mathrm{inc}}\end{pmatrix}\right]_\Gamma.$$

The family of analytic operators $\boldsymbol{A}(s)$ satisfies the following bound for $\operatorname{Re} s>0$,

$$\|\boldsymbol{A}(s)\|_{\mathrm{X}_\Gamma^4\leftarrow\mathrm{X}_\Gamma^4}\leq C(\varepsilon,\mu,\Gamma)\,\frac{|s|^2+1}{\operatorname{Re} s}+\frac{1}{2},$$

where $C(\varepsilon,\mu,\Gamma)$ depends on bounds of the physical functions ε, μ and the boundary Γ. Moreover, the boundary integral operator inherits the coercivity property from the Calderón operator. More precisely, for $\operatorname{Re} s>0$ the bound (1.19) holds, when $\boldsymbol{C}_{\varepsilon,\mu}(s)$ is replaced by $\boldsymbol{A}(s)$. With boundedness and coercivity, we employ the Lax-Milgram theorem to obtain a bounded inverse operator of (1.22). More precisely, the BIE has the unique solution

$$\begin{pmatrix}\widehat{\boldsymbol{\phi}}^+\\ \widehat{\boldsymbol{\phi}}^-\end{pmatrix}=\boldsymbol{A}(s)^{-1}\begin{pmatrix}-\widehat{\boldsymbol{g}}^{\mathrm{inc}}\\ \widehat{\boldsymbol{g}}^{\mathrm{inc}}\end{pmatrix}\in\mathrm{X}_\Gamma^4, \tag{1.23}$$

and $\boldsymbol{A}(s)^{-1}$ satisfies the bound

$$\|\boldsymbol{A}(s)^{-1}\|_{\mathrm{X}_\Gamma^4\leftarrow\mathrm{X}_\Gamma^4}\leq C(\varepsilon,\mu,\Gamma)\,\frac{|s|^2+1}{\operatorname{Re} s}, \tag{1.24}$$

where $C(\varepsilon,\mu,\Gamma)$ depends on bounds of the physical functions ε, μ and the boundary Γ. From this equation, we can clearly see, that traces $\widehat{\boldsymbol{g}}^{\mathrm{inc}}$ of the given incoming electromagnetic fields can be mapped by a bounded linear operator $\boldsymbol{A}(s)^{-1}$ to the tangential traces of the desired scattered fields $\widehat{\boldsymbol{\phi}}^+$ and $\widehat{\boldsymbol{\phi}}^-$, see (1.21).

Next, we concatenate the representation formula (1.17) with the inverse boundary integral operator. The composed operator is denoted by $\boldsymbol{\mathcal{U}}^\pm(s)$. We point out, that $\boldsymbol{\mathcal{U}}^\pm$ maps the given time-harmonic incoming traces $\widehat{\boldsymbol{g}}^{\mathrm{inc}}$ to the Laplace transforms $(\widehat{\boldsymbol{E}}^\pm,\widehat{\boldsymbol{H}}^\pm)$ of the desired electromagnetic fields. For further details, see Section 3.6.2. Moreover, we obtain the bound

$$\|\boldsymbol{\mathcal{U}}^\pm(s)\|_{H(\mathbf{curl},\Omega^\pm)^2\leftarrow\mathrm{X}_\Gamma^2}\leq C_\sigma\,\frac{|s|^3}{(\operatorname{Re} s)^{3/2}},\qquad\text{for}\quad\operatorname{Re} s\geq\sigma>0. \tag{1.25}$$

Convolution quadrature The concept of convolution quadrature was first constructed by Lubich for multistep methods and then extended to Runge-Kutta methods, see, e.g., [16]. We make use of a convolution quadrature based on an m-stage implicit Runge–Kutta method, see [63], for the discretization of the initial value problem

$$y' = f(t, y), \qquad y(0) = y_0.$$

Let $\tau > 0$ be the time stepsize and let y^n be the approximation to $y(t_n)$ at time $t_n = n\tau$. Furthermore, let Y^{ni} be the internal stages to approximate $y(t_n + c_i\tau)$, obtained as the solution to

$$\begin{aligned} Y^{ni} &= y^n + \tau \sum_{j=1}^{m} a_{ij} f(t_n + c_j\tau, Y^{nj}), \qquad i = 1, \dots, m, \\ y^{n+1} &= y^n + \tau \sum_{j=1}^{m} b_j f(t_n + c_j\tau, Y^{nj}). \end{aligned}$$

The method is determined by its coefficients

$$\mathscr{A} = (a_{ij})_{i,j=1}^{m}, \quad \boldsymbol{b} = (b_1, \dots, b_m)^T, \quad \text{and} \quad \boldsymbol{c} = (c_1, \dots, c_m)^T,$$

where we always assume that $\mathscr{A}$ is invertible. To construct the convolution quadrature weights, we use the *Runge–Kutta differentiation symbol*

$$\Delta(\zeta) = \Big(\mathscr{A} + \frac{\zeta}{1-\zeta} \mathbb{1}\boldsymbol{b}^T\Big)^{-1} \in \mathbb{C}^{m\times m}, \qquad \zeta \in \mathbb{C} \text{ with } |\zeta| < 1.$$

For example, the well-known implicit Euler method corresponds to the symbol $\Delta_{\text{impEuler}}(\zeta) = 1 - \zeta$. Concerning the wellposedness and eigenvalues of $\Delta(\zeta)$, more information can be found in Chapter 3.

Let $\boldsymbol{X}$, $\boldsymbol{Y}$ be Banach spaces and let $\boldsymbol{K}(s) : \boldsymbol{X} \to \boldsymbol{Y}$ be an analytic family of linear operators for $\operatorname{Re} s \geq \sigma_0 > 0$, such that for $\kappa \in \mathbb{R}$ and $\nu \geq 0$ we have

$$\|\boldsymbol{K}(s)\|_{\boldsymbol{Y}\leftarrow\boldsymbol{X}} \leq M_\sigma \frac{|s|^\kappa}{(\operatorname{Re} s)^\nu}. \tag{1.26}$$

Let $\boldsymbol{g} : [0, T] \to \boldsymbol{X}$ be sufficiently regular and extended to 0 for $t < 0$. The Heaviside notation (1.14) naturally extends to the Banach-space-valued functions, such that the operator $\boldsymbol{K}$ is a convolution operator $\boldsymbol{K}(\partial_t) : H_0^{r+\kappa}(0, T; \boldsymbol{X}) \to \boldsymbol{H}_0^r(0, T; \boldsymbol{Y})$ for arbitrary real r, cf. (1.5). For two compatible operators $\boldsymbol{K}, \boldsymbol{L}$ we have the composition

$$\boldsymbol{K}(\partial_t)\boldsymbol{L}(\partial_t)\boldsymbol{g} = (\boldsymbol{K}\boldsymbol{L})(\partial_t)\boldsymbol{g}. \tag{1.27}$$

To deal with the convolution $\boldsymbol{K}(\partial_t)\boldsymbol{g}$ numerically, we replace the differential calculus ∂_t by a discrete calculus $\partial_t^\tau = \Delta(\zeta)/\tau$ and expand into a generating function, cf. [65],

$$\boldsymbol{K}\Big(\frac{\Delta(\zeta)}{\tau}\Big) = \sum_{n=0}^{\infty} \boldsymbol{W}_n(\boldsymbol{K})\zeta^n.$$

Here, the convolution quadrature "weights" are operators $\boldsymbol{W}_n(\boldsymbol{K}) : \boldsymbol{X}^m \to \boldsymbol{Y}^m$. For the given function $\boldsymbol{g}$, we define the sequence of values $\widetilde{\boldsymbol{g}} = (\widetilde{\boldsymbol{g}}^n)$ with $\widetilde{\boldsymbol{g}}^n = \big(\boldsymbol{g}(t_n + c_i\tau)\big)_{i=1}^m$, adjusted to the Runge–Kutta stages. Then, the discrete convolution of $\boldsymbol{K}$ with $\widetilde{\boldsymbol{g}}$ is given as

$$\big(\boldsymbol{K}(\partial_t^\tau)\widetilde{\boldsymbol{g}}\big)^n = \sum_{j=0}^{n} \boldsymbol{W}_{n-j}(\boldsymbol{K})\widetilde{\boldsymbol{g}}^j \in \boldsymbol{Y}^m.$$

According to [11, Theorem 4.2], we have the approximation property

$$i\text{-th component of the vector } \big(\boldsymbol{K}(\partial_t^\tau)\widetilde{\boldsymbol{g}}\big)^n \quad \approx \quad \big(\boldsymbol{K}(\partial_t)\boldsymbol{g}\big)(t_n + c_i\tau). \tag{1.28}$$

In particular, we use the Radau IIA methods, i.e., $c_m = 1$, such that $t_{n-1} + c_m\tau = t_n$ in (1.28). Consequently, the m-th, i.e., the last component of the vector $\big(\boldsymbol{K}(\partial_t^\tau)\widetilde{\boldsymbol{g}}\big)^{n-1}$ approximates the continuous convolution at t_n,

$$\big(\boldsymbol{K}(\partial_t)\boldsymbol{g}\big)(t_n) \approx \Big[\big(\boldsymbol{K}(\partial_t^\tau)\widetilde{\boldsymbol{g}}\big)^{n-1}\Big]_m \in \boldsymbol{Y}.$$

An important property of the convolution quadrature is that it inherits the composition rule (1.27), which is also true for the continuous convolution. That is, for two analytic families of operators $\boldsymbol{K}(s)$ and $\boldsymbol{L}(s)$ mapping into compatible spaces, the convolution quadrature discretization satisfies, see, e.g., [95, Equation (3.5)],

$$\boldsymbol{K}(\partial_t^\tau)\boldsymbol{L}(\partial_t^\tau)\widetilde{\boldsymbol{g}} = (\boldsymbol{K}\boldsymbol{L})(\partial_t^\tau)\widetilde{\boldsymbol{g}}. \tag{1.29}$$

The composition rule (1.29) is crucial, since it allows us to equivalently discretize the BIE with the inverse operator.

The time discretization for the scattering problem is based on the following error bound for Runge–Kutta convolution quadrature from [15] applied to Radau IIA methods [63, Section IV.5]. We draw attention to the bounds (1.20), (1.24), and (1.25), which are of the same type as (1.26) and play an important role for the next result.

Lemma 1.5 ([15, Theorem 3])**.** *Let $\boldsymbol{K}(s) : \boldsymbol{X} \to \boldsymbol{Y}$, $\operatorname{Re} s > \sigma_0 \geq 0$, be an analytic family of linear operators between Banach spaces $\boldsymbol{X}$ and $\boldsymbol{Y}$ satisfying the bound (1.26) with exponents κ and ν. Consider the Runge–Kutta convolution quadrature based on the Radau IIA method with m stages. Let $1 \leq q \leq m$ (the most interesting case is $q = m$) and $r > \max(2q + \kappa, 2q - 1, q + 1)$. Let $\boldsymbol{g} \in \boldsymbol{C}^r([0,T], \boldsymbol{X})$ satisfy $\boldsymbol{g}(0) = \boldsymbol{g}'(0) = \ldots = \boldsymbol{g}^{(r-1)}(0) = 0$ and let $\widetilde{\boldsymbol{g}}$ be the corresponding sequence of values. Then, the following error bound holds at $t_n = n\tau \in [0,T]$*

$$\begin{aligned}&\Big\|\Big[\big(\boldsymbol{K}(\partial_t^\tau)\widetilde{\boldsymbol{g}}\big)^{n-1}\Big]_m - \big(\boldsymbol{K}(\partial_t)\boldsymbol{g}\big)(t_n)\Big\|_{\boldsymbol{Y}} \\ &\qquad \leq C\, M_{1/T}\, \tau^{\min(2q-1,\, q+1-\kappa+\nu)} \left(\|\boldsymbol{g}^{(r)}(0)\|_{\boldsymbol{X}} + \int_0^t \|\boldsymbol{g}^{(r+1)}(\theta)\|_{\boldsymbol{X}}\, \mathrm{d}\theta\right).\end{aligned}$$

The constant C is independent of τ, $\boldsymbol{g}$, and M_σ of (1.26), but depends on the exponents κ and ν in (1.26) and on the final time T.

Convolution quadrature for the scattering problem At this stage, we return back from the frequency domain to the time domain, employing the Heaviside notation (1.14). To obtain a time-dependent version of the BIE (1.22), we formally insert the differentiation operator ∂_t in place of the frequency variable s. Given $\boldsymbol{g}^{\mathrm{inc}} : [0,T] \to \mathrm{X}_\Gamma^2$, we seek time-dependent boundary densities $(\boldsymbol{\phi}^+, \boldsymbol{\phi}^-) : [0,T] \to \mathrm{X}_\Gamma^2 \times \mathrm{X}_\Gamma^2$ such that

$$\boldsymbol{A}(\partial_t)\boldsymbol{\phi} = \boldsymbol{g} \quad \text{with} \quad \boldsymbol{\phi}(t) = \begin{pmatrix}\boldsymbol{\phi}^+(t)\\ \boldsymbol{\phi}^-(t)\end{pmatrix} \in \mathrm{X}_\Gamma^4, \quad \boldsymbol{g}(t) = \begin{pmatrix}-\boldsymbol{g}^{\mathrm{inc}}(t)\\ \boldsymbol{g}^{\mathrm{inc}}(t)\end{pmatrix} \in \mathrm{X}_\Gamma^4. \tag{1.30}$$

Recall that the inverse operator $\boldsymbol{A}^{-1}(s)$ from (1.23) satisfies the bound (1.24). Employing the Heaviside notation (1.14) and the composition rules $\boldsymbol{A}^{-1}(\partial_t)\boldsymbol{A}(\partial_t) = \mathbf{Id}$ and $\boldsymbol{A}(\partial_t)\boldsymbol{A}^{-1}(\partial_t) = \mathbf{Id}$, we obtain the

unique solution of (1.30) as

$$\boldsymbol{\phi} = \boldsymbol{A}^{-1}(\partial_t)\boldsymbol{g}.$$

We apply the Runge–Kutta based convolution quadrature discretization to the BIE (1.30)

$$\boldsymbol{A}(\partial_t^\tau)\boldsymbol{\phi}_\tau = \boldsymbol{g}, \qquad \text{or equivalently,} \qquad \boldsymbol{\phi}_\tau = \boldsymbol{A}^{-1}(\partial_t^\tau)\,\boldsymbol{g}, \tag{1.31}$$

with $\boldsymbol{\phi}$ and $\boldsymbol{g}$ defined in (1.30). The two equations above are equivalent due to the discrete composition rule (1.29). Then, we obtain the time discretization of the electromagnetic fields by inserting the boundary densities from (1.31) into the representation formulas (1.17) and applying the convolution quadrature.

Recall the time-harmonic representation operator $\boldsymbol{\mathcal{U}}^\pm$, which concatenates the representation formula (1.17) with the inverse boundary integral operator. Applying the composition rule (1.27) yields a representation operator $\boldsymbol{\mathcal{U}}^\pm(\partial_t)$ for the solution to the time-dependent scattering problem (1.13). Crucially, with the discrete composition rule (1.29), it is equivalent to apply the convolution quadrature $\boldsymbol{\mathcal{U}}^\pm(\partial_\tau)$ to the given incoming boundary traces $\boldsymbol{g}^{\mathrm{inc}}$, or to apply convolution quadrature $\boldsymbol{A}^{-1}(\partial_\tau)$ to $\boldsymbol{g}$ and apply another convolution quadrature and the representation formula (1.17).

In the upcoming theorem, we apply an $m-$stage Radau IIA convolution quadrature for the time discretization and k-th order Raviart–Thomas boundary elements for the space discretization, cf. [119]. We find that, in general, we obtain an order reduction on $\Omega^\pm$. However, in [113], we show, that on a domain $\Omega_d^\pm = \{x \in \Omega \,|\, \operatorname{dist}(x,\Gamma) > d\}$ with $d > 0$, away from the boundary, we have full-order convergence. This stems from an improved bound with respect to the frequency variable s. This bound decays exponentially in $\operatorname{Re} s$, which dominates any polynomial growth in s.

Theorem 1.6 (Error bound of the full discretization)**.** *Consider the time-dependent scattering problem (1.13) and let $\boldsymbol{g} \in H_0^{r+3}(0,T;\mathrm{X}_\Gamma^4)$ for some arbitrary $r \geq 0$.*
For $r > 2m+4$ we assume the incoming waves to satisfy $\boldsymbol{g} \in \boldsymbol{C}^r([0,T],\mathrm{X}_\Gamma^4)$. Moreover, we assume $\boldsymbol{g}$ to vanish at $t=0$ together with its first $r-1$ time derivatives. Furthermore, it is assumed that the solution $\boldsymbol{\phi}$ of the boundary integral equation (1.30) is sufficiently regular and vanishes at $t=0$ together with its time derivatives.
Let τ be the time stepsize and h the mesh width of the k-th order boundary element discretization. Then, the approximations to the electromagnetic fields at time t_n, both in the interior and the exterior domain,

$$\left(\boldsymbol{E}_{\tau,h}^\pm\right)^n = \left[(\boldsymbol{E}_{\tau,h}^\pm)^{n-1}\right]_m \quad \text{and} \quad \left(\boldsymbol{H}_{\tau,h}^\pm\right)^n = \left[(\boldsymbol{H}_{\tau,h}^\pm)^{n-1}\right]_m,$$

satisfy the following error bound of order $m-1/2$ in time and order $k+3/2$ in space at $t_n = n\tau \in [0,T]$:

$$\left\|\left(\boldsymbol{E}_{\tau,h}^\pm\right)^n - \boldsymbol{E}(t_n)\right\|_{H(\mathbf{curl},\Omega^\pm)} + \left\|\left(\boldsymbol{H}_{\tau,h}^\pm\right)^n - \boldsymbol{H}(t_n)\right\|_{H(\mathbf{curl},\Omega^\pm)} \leq C\big(\tau^{m-1/2} + h^{k+3/2}\big).$$

For $r > 2m+4$, we obtain the full order $2m-1$ in time away from the interface Γ, on the domains $\Omega_d^\pm = \{x \in \Omega : \operatorname{dist}(x,\Gamma) > d\}$ with $d > 0$, which reads

$$\left\|\left(\boldsymbol{E}_{\tau,h}^\pm\right)^n - \boldsymbol{E}(t_n)\right\|_{\boldsymbol{C}^1(\overline{\Omega}_d^\pm)^3} + \left\|\left(\boldsymbol{H}_{\tau,h}^\pm\right)^n - \boldsymbol{H}(t_n)\right\|_{\boldsymbol{C}^1(\overline{\Omega}_d^\pm)^3} \leq C_d\big(\tau^{2m-1} + h^{k+3/2}\big).$$

The constants C and C_d are independent of n, τ, and h, but depend on the final time T and on the regularity of the incoming traces $\boldsymbol{g}$ and $(\boldsymbol{\varphi},\psi)$ as stated. C_d additionally depends on the distance d.

The motivation for the problem formulation summarized here (see Chapter 3 and [113]) builds on [38], where the authors provide a numerical analysis for time-dependent electromagnetic scattering from dielectric penetrable obstacles. Our contribution is the rigorous numerical analysis of a scattering problem from dispersive materials, which are modeled by nonlocal convolutional material laws in the time domain and frequency-dependent permittivities and permeabilities ε and μ in the Laplace domain. In contrast to previous papers, the functions ε and μ are not set to constants, but depend on the frequency variable. The extension to nonlocal materials inside and outside of the scatterer can be carried out in a straightforward way. A major challenge in this work involved finding an appropriate problem formulation that balances the modeling of physically relevant assumptions for dispersive materials, and also leads to wellposedness of the corresponding BIEs. Furthermore, we provide the first numerical approximation scheme for time-dependent electromagnetic scattering from dispersive materials based on time-dependent boundary integral equations, together with a rigorous error analysis. The techniques that we used here were originally applied to the analogue acoustic problem setting without nonlocal materials, cf. [18, 19], and further developed in [84, 112] for the electromagnetic case.

1.4 Results of implicit-explicit scheme for semilinear and nonlocal wave equations with kinetic b.c.

The viscoacoustic wave equation is given by

$$\partial_{tt}u(t) - c^2\Delta u(t) + \int_{-\infty}^{t} b(t-\theta)\Delta u(\theta)\,\mathrm{d}\theta = f_\Omega(t,u), \qquad u(0)=u_0, \quad u_t(0)=v_0, \qquad \text{on } \Omega, \tag{1.32a}$$

where $\Omega \subset \mathbb{R}^d$ is a bounded domain with smooth boundary Γ, and for $\theta < 0$ we set $u(\theta) = u_0$. It is a well-established equation for describing the impact of a mechanical-energy wave to a nonlocal material. The material may show dissipation and memory at the same time, cf. [101]. Nonlocality refers to materials, where the material's response is not immediate. Instead, its recent history plays a major role. We say that the material has a memory. The dependence on the past is modeled by a convolution. The convolution kernel b is determined by physical properties and describes the viscosity of the material.

In applications, wave propagation is often modeled with dynamic boundary conditions. That is, the wave solves another differential equation on the boundary. An example is a vibrating membrane being disturbed by linear tension and with nonvanishing mass density, see [54, Sec. 5&6], [91, S.56]. This can be described by kinetic boundary conditions with $d = 2$. Another application of kinetic boundary conditions can be found in [107, Sec. 3.2]. It models the membrane of a bass drum with a hole in the interior and thick border.

We equip (1.32a) with kinetic boundary conditions, i.e., on Γ we require the solution to solve

$$\partial_{tt}u(t) - c^2\Delta_\Gamma u(t) + c^2\boldsymbol{n}\cdot\nabla u + \int_{-\infty}^{t} b(t-s)\Delta_\Gamma u(s)\,\mathrm{d}s - \int_{-\infty}^{t} b(t-s)\boldsymbol{n}\cdot\nabla u(s)\,\mathrm{d}s = f_\Gamma(t), \tag{1.32b}$$

with the Laplace-Beltrami operator Δ_Γ defined in (1.2). To simplify the presentation, we define the extended Laplace operator

$$\Delta_{\Omega,\Gamma} = \begin{cases} \Delta, & \text{in} \quad \Omega, \\ \Delta_\Gamma - \boldsymbol{n}\cdot\nabla, & \text{on} \quad \Gamma. \end{cases}$$

Thus, with $f = (f_\Omega, f_\Gamma)$ we abbreviate (1.32) as,

$$\partial_{tt}u(t) - c^2\Delta_{\Omega,\Gamma}u(t) + \int_{-\infty}^{t} b(t-s)\Delta_{\Omega,\Gamma}u(s)\mathrm{d}s = f(t,u), \qquad u(0)=u_0, \quad u_t(0)=v_0. \tag{1.33a}$$

In the preprint [32], we provide a general framework which covers Dirichlet conditions as well. However, in this short summary, we focus on kinetic boundary conditions and therefore use the bulk-surface Sobolev spaces defined in (1.1).

In a common model studied in geophysical literature, e.g., [34, Chap. 2] and [68], the kernel b is given by a linear combination of exponentials. For convenience, we only consider the case of a single exponential kernel in this summary, i.e.,

$$b(t) = \beta \mathrm{e}^{-\lambda t}, \qquad \beta, \lambda > 0. \tag{1.33b}$$

The setting can be transferred to the case of multiple kernels. The exponential kernel controls how the past influences the present. More precisely, more recent states have a greater impact on the material than the history lying further away in the past, cf. [34, Sec. 2.1.1]. The material has a fading memory.

From a numerical point of view, the viscoacoustic wave equation with kinetic boundary conditions is challenging for two major reasons. First, the additional convolution makes standard time integration

schemes unfeasible, since we would have to keep track of all former values, resulting in large storage requirements. Second, the kinetic boundary condition is posed on a smooth boundary, such that, in general, a standard polygonal space discretization can not approximate the boundary correctly. This leads to the difficulty that the numerical approximation does not live on the same spatial domain as the exact solution, meaning the approximation space is not a subset of the space containing the exact solution. Consequently, the comparison of the exact solution and the numerical approximation is more involved. Then, a lift operator from the approximation space to the exact space can be used, cf. [76, 77, 91].

To avoid a huge storage for the time discretization, we replace the convolution by an additional variable, called the auxiliary memory variable. Due to the exponential kernels (1.33b), the memory variable solves a first-order differential equation, which can be coupled to the first-order system of the wave equation. However, it is not trivial to find a suitable definition of the memory variable to obtain wellposedness. In [51], the author uses an evolution equation setting and interprets the memory variable as a bounded or sufficiently small relatively bounded perturbation to a wave-type operator. However, in our situation, this is not possible, due to the Laplace operator acting on the convolution. We follow the literature [2] and perform a shift in the convolution, to obtain

$$\int_{-\infty}^{t} \beta \mathrm{e}^{-\lambda(t-\theta)} \Delta_{\Omega,\Gamma} u(\theta)\,\mathrm{d}\theta = \frac{\beta}{\lambda}\Delta_{\Omega,\Gamma} u(t) - \beta \Delta_{\Omega,\Gamma} M(t),$$

with the auxiliary variable

$$M(t) = \int_{-\infty}^{t} \mathrm{e}^{-\lambda(t-\theta)} \big(u(t) - u(\theta)\big)\,\mathrm{d}\theta, \qquad t \geq 0.$$

Taking the derivative with respect to time of the auxiliary variable M and calculating the remaining integral, we couple the additional differential equation to the wave equation and obtain the first-order in time coupled PDE,

$$\begin{aligned} \partial_t u &= v, & u(0) &= u_0, & \\ \partial_t v &= \alpha \Delta_{\Omega,\Gamma} u + \beta \Delta_{\Omega,\Gamma} M + f, & v(0) &= v_0, & \alpha &= c^2 - \frac{\beta}{\lambda}, \\ \partial_t M &= -\lambda M + \frac{1}{\lambda} v, & M(0) &= 0. & \end{aligned}$$

We write (1.34) in an evolution equation setting,

$$x' + \mathcal{A}x = F,$$

where

$$x = \begin{pmatrix} u \\ v \\ M \end{pmatrix}, \qquad \mathcal{A} = \begin{pmatrix} 0 & -\mathrm{I} & 0 \\ -\alpha\Delta_{\Omega,\Gamma} & 0 & -\beta\Delta_{\Omega,\Gamma} \\ 0 & -\frac{1}{\lambda} & \lambda \end{pmatrix}, \qquad F = \begin{pmatrix} 0 \\ f \\ 0 \end{pmatrix}.$$

To show that (1.35) is well-posed in a suitable space X and for a sufficiently regular right-hand side f, we employ the Lumer-Phillips theorem. To this end, we show monotonicity, i.e., there exists a constant c_m such that

$$\big(\mathcal{A}x, x\big)_X \geq -\mathrm{c}_m \|x\|_X^2, \tag{1.36}$$

where $\mathrm{c}_m = 0$ for homogeneous Dirichlet boundary conditions and $\mathrm{c}_m > \frac{1}{2}$ is sufficiently large, depending on the parameters α, β and λ, for kinetic boundary conditions. To obtain the monotoncity (1.36) we add

the weights α and $\mu = \beta\lambda > 0$ to the canonical space $H^1(\Omega,\Gamma) \times L^2(\Omega,\Gamma) \times H^1(\Omega,\Gamma)$. Now, using [115], it follows that the monotone operator $\mathcal{A}$ generates a contractive, strongly continuous semigroup on the Hilbert space,

$$X = H^1_\alpha(\Omega,\Gamma) \times L^2(\Omega,\Gamma) \times H^1_\mu(\Omega,\Gamma).$$

For the right-hand side f we require sufficient regularity and that it fulfills a growth condition, such that a local Lipschitz property follows from a Sobolev embedding theorem. Thus, in contrast to the stiff linearity $\mathcal{A}$, the right-hand side has the property of being locally Lipschitz. This will be exploited for the efficiency of the numerical time stepping, which we introduce next.

Let $\tau > 0$ be the time stepsize. For the discretization of the differential equation of M, we introduce the notation

$$\gamma_\pm = 1 \pm \frac{\tau\lambda}{2}, \qquad \gamma = \frac{\gamma_-}{\gamma_+}.$$

Furthermore, we denote the modified scalars

$$\widetilde{\alpha} = \left(\alpha + \frac{\beta}{\lambda\gamma_+}\right) > \alpha, \quad \text{and} \quad \widetilde{\beta} = \frac{\beta(1+\gamma)}{2} \in [0,\beta).$$

The implicit-explicit (IMEX) time discretization scheme is constructed by combining the Crank-Nicolson with the leapfrog scheme, cf. [77, Section 2.2.]. For $n \in \mathbb{N}$, we abbreviate $t_n = n\tau$ and $f^n = f(t_n, u^n)$ for the evaluation of the right-hand side at the numerical approximation $u^n \approx u(t_n)$. We denote

$$\mathbf{\Phi}_{\Omega,\Gamma,\tau}(u,v,M) = \frac{\tau}{2}\Delta_{\Omega,\Gamma}\big(\alpha u + \widetilde{\beta}M\big) + \frac{\tau^2}{4}\widetilde{\alpha}\Delta_{\Omega,\Gamma}v$$

and formulate the IMEX scheme in a half-step formulation

$$v^{n+\frac{1}{2}} = v^n + \mathbf{\Phi}_{\Omega,\Gamma,\tau}\big(u^n, M^n, v^{n+\frac{1}{2}}\big) + \frac{\tau}{2}f^n, \tag{1.37a}$$

$$\begin{aligned} u^{n+1} &= u^n + \tau v^{n+\frac{1}{2}}, \\ M^{n+1} &= \gamma M^n + \gamma_+^{-1}\frac{\tau}{\lambda}v^{n+\frac{1}{2}}, \end{aligned}$$

$$v^{n+1} = v^{n+\frac{1}{2}} + \mathbf{\Phi}_{\Omega,\Gamma,\tau}\big(u^n, M^n, v^{n+\frac{1}{2}}\big) + \frac{\tau}{2}f^{n+1}. \tag{1.37b}$$

Note that $\mathbf{\Phi}_{\Omega,\Gamma,\tau}$ appears in the same way in the half and the full steps, (1.37a) and (1.37b). Subtracting (1.37a) and (1.37b) gives an equivalent and computationally more efficient way to obtain v^{n+1}, see also [77, Remark 2.6]. Hence we have

$$v^{n+1} = -v^n + 2v^{n+1/2} + \frac{\tau}{2}(f^{n+1} - f^n).$$

We note that in the above scheme (1.37), the stiff linear part, which corresponds to $\mathcal{A}$, is treated implicitly in order to avoid severe stepsize restrictions for fine meshes. For the Crank-Nicolson scheme, the time stepping for the inhomogeneity would be $\frac{\tau}{4}(f^n + f^{n+1})$ for both v^{n+1} and $v^{n+\frac{1}{2}}$, leading to a nonlinear system to be solved in each update step. A remarkable advantage of the rearrangement is, that the right-hand side is only evaluated at previously calculated approximations. This makes the IMEX scheme more efficient, since only linear systems need to be solved. The wellposedness of the IMEX scheme can be shown by an induction.

The error analysis of the IMEX scheme crucially exploits the fact, that it can be written into an equivalent first-order formulation

$$x^{n+1} = Rx^n + \frac{\tau}{2}R_+^{-1}y^n + \frac{\tau^2}{4}R_+^{-1}z^n, \qquad \text{where} \qquad R_\pm = \mathrm{Id} \pm \frac{\tau}{2}\mathcal{A}, \qquad R = R_+^{-1}R_-, \tag{1.38a}$$

and

$$y^n = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} (f^n + f^{n+1}), \qquad z^n = \begin{pmatrix} 1 \\ 0 \\ \frac{1}{\lambda} \end{pmatrix} (f^n - f^{n+1}). \tag{1.38b}$$

This allows the interpretation of the IMEX scheme as a perturbation of the Crank-Nicolson scheme. To show an error bound for the IMEX scheme, we first insert the exact solution into the IMEX scheme, which yields a provably stable error recursion. Afterwards, we bound the occurring defects.

We briefly discuss the main difficulties in bounding the defects. Since we interpret the IMEX scheme as a perturbation of the Crank-Nicolson scheme, the IMEX defect $\delta^\ell_{\mathrm{IMEX}} = \delta^\ell_{\mathrm{CN}} + \widetilde{\delta}^\ell$ in each step $\ell \in \mathbb{N}$ of the error recursion consists of a Crank-Nicolson defect and an additional perturbation defect $\widetilde{\delta}$. While the Crank-Nicolson defect is easily bounded of order $\mathcal{O}(\tau^3)$, the additional defect $\widetilde{\delta}^\ell$ is more tricky. We denote by $\widetilde{\ }$ the exact evaluation, then we follow [91, p. 41] and split $\widetilde{\delta}^\ell$ into two parts

$$\widetilde{\delta}^{\ell+1} = \widetilde{\delta}_1^{\ell+1} + \widetilde{\delta}_2^{\ell+1} \qquad \text{with} \qquad \widetilde{\delta}_1^{\ell+1},\ \widetilde{\delta}_2^{\ell+1} \ \in\ \mathcal{O}\big(\tau(\widetilde{f}^\ell - \widetilde{f}^{\ell+1})\big).$$

The difference $\tau(\widetilde{f}^\ell - \widetilde{f}^{\ell+1})$ is of order $\mathcal{O}(\tau^2)$, which is insufficient due to the summation for the global error, leading to the loss of one order of τ. The important step towards a second-order convergence is the combination of two defects for two different time steps to gain an extra order of τ, i.e., with R from (1.38), we arrive at

$$\widetilde{\delta}_1^{\ell+1} + R\widetilde{\delta}_2^{\ell} \ \in\ \mathcal{O}\big(\tau(\widetilde{f}^{\ell-1} - 2\widetilde{f}^{\ell} + \widetilde{f}^{\ell+1})\big).$$

Then, recovering the finite difference quotient, we have the bound $\tau \left\| \widetilde{f}^{\ell-1} - 2\widetilde{f}^{\ell} + \widetilde{f}^{\ell+1} \right\|_{L^2(\Omega,\Gamma)} \le C\tau^3$, which leads to the desired global second-order error bound.

Theorem 1.7 (Error bound IMEX scheme)**.** *Assume that the solution $x = (u, v, M)$ of (1.34) satisfies $u \in C^4([0,T], L^2(\Omega,\Gamma)) \cap C^3([0,T], H^1(\Omega,\Gamma))$ and $\alpha u + \beta M \in C^2([0,T], H^2(\Omega,\Gamma))$ and that $\tau > 0$ is sufficiently small. Then, the approximation $x^n \approx x(t_n)$, $t_n = n\tau$ given in (1.37) satisfies the error bound*

$$\|x^n - x(t_n)\|_X \le C\mathrm{e}^{Kt_n}\tau^2,$$

where $K = \mathrm{c}_m + \frac{L_f(1+\sqrt{2})}{\sqrt{\alpha} - L_f\tau(1+\sqrt{2})}$. The constant C only depends on u and T, and L_f is the local Lipschitz constant of f.

The main contribution of this work is the construction and the rigorous error analysis of a new IMEX scheme for a wave equation that includes a nonlocal-in-time material law and is equipped with kinetic boundary conditions. We provide a uniform second-order error bound for the time discretization. Compared to the setting in [77], the block structure of the operator in the first-order formulation has at least three components, making calculations more involved than in [77]. Moreover, defining the auxiliary variable which leads to a well-posed evolution equation needs proper considerations. In particular, we included an adequate shift, cf. [2], and derived a framework using weighted Sobolev spaces.

Outlook The full discretization, which has not been treated here, is a direct combination of isoparametric finite elements, cf. [46], which are suitable for a smooth boundary Γ, with the error analysis presented here. More precisely, we perform the IMEX scheme and its error analysis in the space of isoparametric finite elements, as indicated for the method of lines.

For more general convolution kernels, we can consider convolution quadrature. In this case, the admissible convolution kernels as well as the convergence are determined by stability of the Laplace transformed equation. In particular, it will be possible to allow for fractional kernels, cf. [101]. However, this is out of the scope of this thesis.

CHAPTER 2

Variational Gaussian approximation for the magnetic Schrödinger equation

The content of the following chapter was published in the Journal of Physics. A., cf. [31]. Here, we added several details of calculations, which are marked in the color grey.

The authors of this paper are Selina Burkhard, Benjamin Dörich, Marlis Hochbruck and Caroline Lasser[1].

In the present chapter we consider the semiclassical magnetic Schrödinger equation, which describes the dynamics of particles under the influence of a magnetic field. The solution of the time-dependent Schrödinger equation is approximated by a single Gaussian wave packet via the time-dependent Dirac–Frenkel variational principle. For the approximation we derive ordinary differential equations of motion for the parameters of the variational solution. Moreover, we prove L^2-error bounds and observable error bounds for the approximating Gaussian wave packet.

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2.1 Introduction

In the present paper we study the semiclassical magnetic Schrödinger equation

$$\mathrm{i}\varepsilon\partial_t\psi(t) = H(t)\psi(t), \quad \psi(0) = \psi_0, \quad t \in \mathbb{R}, \tag{2.1a}$$

on $\mathbb{R}^d$ with magnetic Hamiltonian

$$H(t) = \frac{1}{2}\big(\mathrm{i}\varepsilon\nabla_x + A(t,x)\big)^2 + V(t,x), \tag{2.1b}$$

and initial value $\psi_0 \in L^2(\mathbb{R}^d)$ with semiclassical parameter $0 < \varepsilon \ll 1$. Here, A is a magnetic vector potential, and V is the electric potential. This equation arises in the modeling of the quantum dynamics of nuclei in a molecule subject to external magnetic fields, cf. [6, 7] or [58, Sec. 4.3.]. From a numerical point of view, solving this time-dependent partial differential equation raises three major problems. First, it is a high-dimensional problem, since the space dimension is typically given by $d = 3N$, where N is the number of nuclear particles in the system. Further, the computational domain $\mathbb{R}^d$ is naturally unbounded, and thus most numerical methods require truncation before discretization. For the method of lines (first discretize space, then time), high dimension combined with an unbounded domain leads to inadequately if not unattractably large systems that have to be integrated in time. Another challenge is given by the high oscillations induced by the small semiclassical parameter ε. For standard time integration schemes severe stepsize restrictions have to be imposed and leave these methods impracticable.

We consider the case that the initial value ψ_0 is strongly localized and given by a Gaussian wave packet,

$$\psi_0(x) = \exp\Big(\frac{\mathrm{i}}{\varepsilon}\big(\frac{1}{2}(x-q)^T\mathcal{C}(x-q) + (x-q)^T p + \zeta\big)\Big),$$

where $q, p \in \mathbb{R}^d$ are the packet's position and momentum center, $\mathcal{C} \in \mathbb{C}^{d\times d}$ is the width matrix of the envelope, and $\zeta \in \mathbb{C}$ a phase and weight parameter. For $A = 0$ it is well established that it is possible to reasonably approximate the solution by a Gaussian wave packet with parameters that are evolved according to ordinary differential equations. First studies in this direction are due to K. Hepp [71] and G. Hagedorn [59] from the perspective of mathematical physics, and E. Heller [69, 70] as well as R. Coalson, M. Karplus [41] with already an eye on numerical computation. The evolution equations for the parameters of all Gaussian wave packet approximations can be classified in two categories:

Variational: The variational approach relies on the time-dependent Dirac–Frenkel principle for deriving the parameter equations of motion. By the variational construction, the Gaussian wave packet automatically inherits several conservation properties of the exact solution.

Semiclassical: The semiclassical approach expands the wave packet ansatz with respect to the semiclassical parameter ε and derives ε independent parameter equations by matching terms with the same order.

Both types of ordinary differential equations have the advantageous property, that their solutions are non-oscillatory. Both approximations have the same convergence order with respect to the semiclassical parameter ε in L^2-norm, and both reproduce the exact solution for the special case of Schrödinger operators with linear magnetic potential A and quadratic electric potential V. For a further discussion, we refer to [35, Chapter 10.2] for a monograph that covers the semiclassical construction, to [98, Chapter II.4] or [87, Chapter 3] for a short book and a review presenting the variational case, and to [127] for a general presentation of Gaussian wave packet dynamics.

Gaussian	L^2-norm	observables
semiclassical	$\mathcal{O}(\sqrt{\varepsilon})$	$\mathcal{O}(\varepsilon)$
variational	$\mathcal{O}(\sqrt{\varepsilon})$	$\mathcal{O}(\varepsilon^2)$

Table 2.1: Error bounds for the semiclassical and the variational approximation of magnetic Schrödinger dynamics according to Theorem 2.13 and Theorem 2.15. The variational observable error estimate extends and improves previously known results.

Contributions of the paper

Our main contribution in this paper is to first show that for the magnetic Schrödinger equation the variational approximation is still given by a system of ordinary differential equations for the parameters defining the Gaussian wave packet. Second, we prove rigorous error bounds for this approximation on finite time intervals $[0, T]$ in terms of the semiclassical parameter ε. The presented results generalize the bounds established in [87, 98] to non-vanishing magnetic potentials A and further allow for time-dependencies in both the electric and the magnetic potential. We also treat the more general case where the dynamics are generated by the Weyl quantization of a smooth and subquadratic Hamiltonian function. This includes convergence in the L^2-norm with order $\mathcal{O}(\sqrt{\varepsilon})$ as well as for expectation values of observables, which resemble certain measurable physical quantities of the wave function, with order $\mathcal{O}(\varepsilon^2)$. These estimates extend and improve the observable bound of [87, Theorem 3.5] and the result of [114] from the case of vanishing magnetic potential. Let us point out that the design and the analysis of time integrators for the magnetic variational equations of motion are currently under investigation, in particular for the numerical simulation of magnetotunneling.

Further wave packet results for $A = 0$

Hagedorn wave packets [59–61] are a multivariate anisotropic generalization of the Hermite functions. They are Gaussian wave packets with a polynomial prefactor, such that a family of them constitutes an orthonormal basis of $L^2(\mathbb{R}^d)$. In [21, 49, 55], time splitting integrators for Hagedorn wave packet approximations are proposed, that combine parameter propagation by ordinary differential equations with a Galerkin step. A spawning method for several families of Hagedorn wave packets is introduced in [121]. For variational Gaussian wave packets, a time splitting integrator, which is robust in the semiclassical parameter ε, is proposed in [48]. Recently in [114], T. Oshawa has analysed the expectation values of position and momentum for a variational Gaussian wave packet and proved $\mathcal{O}(\varepsilon^{3/2})$ accuracy. Our results here generalize and improve this error bound in two ways: First, we allow for general sublinear observables. Second, our method of proof shows $\mathcal{O}(\varepsilon^2)$ observable accuracy also for the case $A \neq 0$. It is worthwhile emphasizing, that from the perspective of the observable error variational Gaussians are more accurate than their semiclassical counterparts.

Related wave packet results for $A \neq 0$

The most general result for the semiclassical wave packet approach is given in [122, Theorem 21] of the monograph by D. Robert and M. Combescure. There, the propagation of Gaussian and Hagedorn

wave packets is covered for a general class of time-dependent Hamiltonian operators $H(t)$, that includes the magnetic Schrödinger operator. The error analysis is with respect to the L^2-norm, but not for observables. The semiclassical construction there also receives corrections, such that it can be accurate to order $\mathcal{O}(\varepsilon^{k/2})$ for any $k \geq 1$. In [23], magnetic Schrödinger operators with polynomially bounded, time-independent magnetic fields and zero potential are considered. The initial coherent state has zero initial energy and its propagation is analysed for the long-time horizon $[0, T/\varepsilon]$. In [83], N. King and T. Ohsawa derive the equations of motion for variational Gaussians in the presence of a magnetic field. They conduct numerical experiments for the expectation value of the position and the momentum operator suggesting that the variational Gaussians are more accurate than the semiclassical ones. An extension of the Hagedorn Galerkin method [49] to the case of magnetic Schrödinger equations is studied in [135], including an error analysis with respect to the L^2-norm. However, no error bounds for the observables are investigated there. For linear magnetic potentials of a particular structure, in [57] a problem adapted splitting method for Hagedorn wave packets is derived but without error analysis. A slightly different approach, called the Gaussian wave packet transform, is proposed for the magnetic Schrödinger equation in [136]. There, the ordinary differential equations for the Gaussian parameters are the semiclassical ones except for an additional term for the scalar parameter ζ.

Outline of the paper

The rest of the paper is structured as follows. For our error analysis we introduce the analytical framework and the variational Gaussian wave packet ansatz in Section 2.2. We present our main results for the magnetic Schrödinger equation in Section 2.3, including the equations for the parameters, the conservation of different quantities, the convergence in the L^2-norm and the convergence of the observables. The proofs of the corresponding results are given in Sections 2.4 to 2.7.

Notation

Throughout the paper, we denote by $L^p(\mathbb{R}^d)$ the classical Lebesgue spaces, and by $\mathcal{S}(\mathbb{R}^d)$ the Schwartz space of rapidly decreasing functions. Further, we make use of the multiindex notation and let for $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}_0^d$, $x \in \mathbb{R}^d$, $f \in \mathcal{S}(\mathbb{R}^d)$

$$|\alpha| \coloneqq \alpha_1 + \ldots + \alpha_d, \qquad x^\alpha \coloneqq x_1^{\alpha_1} \ldots x_d^{\alpha_d}, \qquad \partial^\alpha f \coloneqq \partial_1^{\alpha_1} \ldots \partial_d^{\alpha_d} f.$$

For a function $W \colon \mathbb{R}^d \to \mathbb{R}^L$, $L \geq 1$, we define the average

$$\langle W \rangle_u \coloneqq \langle u | W u \rangle = \int_{\mathbb{R}^d} W(x) |u(x)|^2 \, \mathrm{d}x,$$

if the integral exists. For a linear operator $\mathbf{A}$ acting on $L^2(\mathbb{R}^d)$, we denote

$$\langle \mathbf{A} \rangle_u \coloneqq \langle u | \mathbf{A} u \rangle = \int_{\mathbb{R}^d} \overline{u(x)} (\mathbf{A}u)(x) \, \mathrm{d}x,$$

whenever the integral is well-defined. We also use the dot product of $v, w \in \mathbb{C}^L$ as $v \cdot w \coloneqq v^T w = v_1 w_1 + \cdots + v_L w_L$.

2.2 General setting

We first discuss the analytic framework for our analysis and introduce the Gaussian wave packets. We further call some results on the wellposedness from the literature. For the vector potential we choose the Coulomb gauge, i.e., $\operatorname{div} A = 0$. In order to shorten notation, we rewrite the Hamiltonian in (2.1b) as

$$H(t) = -\frac{\varepsilon^2}{2}\Delta + \mathrm{i}\varepsilon A(t)\cdot\nabla + \widetilde{V}(t), \qquad \widetilde{V} := \frac{1}{2}|A|^2 + V. \tag{2.2}$$

Assumption 2.1. *The scalar potential $\widetilde{V}\colon \mathbb{R}\times\mathbb{R}^d \to \mathbb{R}$ and the vector valued potential $A = (A_j)_{j=1,\dots,d}\colon \mathbb{R}\times\mathbb{R}^d \to \mathbb{R}^d$ are infinitely often differentiable and in addition*

(a) *$\widetilde{V}$ is subquadratic, i.e. $\nabla^k\widetilde{V}$ is bounded for all $k \geq 2$, and*

(b) *A is sublinear, i.e. $\nabla^k A$ is bounded for all $k \geq 1$, and satisfies $\operatorname{div} A = 0$.*

If in addition to Assumption 2.1, we assume that $\partial_t A$ is sublinear, then it can be shown that the initial value problem (2.1a) is well-posed for initial values in L^2, cf. [134, sec. 4] or the remarks after [122, Def. 1] or [104, Rem. 5.14]. In particular, the following wellposedness result on the unitarity of the time evolution guarantees that the norm of the solution of (2.1a) is the same as the one of the initial data. However, for our analysis here, only Assumption 2.1 will be used.

Theorem 2.2 ([134, sec. 4])**.** *Let Assumption 2.1 hold and assume that $\partial_t A$ is sublinear. There exists a unitary evolution family $(U(t,s))_{t,s\in\mathbb{R}}$ on $L^2(\mathbb{R}^d)$ such that for all initial data $\psi_0 \in L^2(\mathbb{R}^d)$ the solution ψ of (2.1a) is given by*

$$\psi(t) = U(t,0)\psi_0. \tag{2.3}$$

In the case of time-independent potentials the evolution family $(U(t,s))_{t,s\in\mathbb{R}}$ reduces to the unitary group $(e^{-it/\varepsilon H})_{t\in\mathbb{R}}$ on $L^2(\mathbb{R}^d)$, which which is given by the spectral theorem and commutes with the Hamiltonian.

Following [87, Chapter 3], we approximate the solution ψ of (2.1a) in the manifold $\mathcal{M}$ of Gaussian wave packets given by

$$\begin{aligned}\mathcal{M} = \Big\{ g \in L^2(\mathbb{R}^d) \;\Big|\; g(x) = \exp\Big(\frac{\mathrm{i}}{\varepsilon}\big(\frac{1}{2}(x-q)^T\mathcal{C}(x-q) + (x-q)^T p + \zeta\big)\Big),\\ q,\, p \in \mathbb{R}^d,\, \mathcal{C} = \mathcal{C}^T \in \mathbb{C}^{d\times d},\, \operatorname{Im}\mathcal{C} \text{ positive definite}, \zeta \in \mathbb{C}\Big\}.\end{aligned} \tag{2.4}$$

The approximating Gaussian wave packet is characterized by the Dirac–Frenkel variational formulation, cf. [87, 98]: seek $u(t) \in \mathcal{M}$ such that for all $t \in \mathbb{R}$ it holds

$$\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}, \quad \big\langle \mathrm{i}\varepsilon\partial_t u(t) - H(t)u(t) \big| v\big\rangle = 0 \quad \text{for all} \quad v \in \mathcal{T}_{u(t)}\mathcal{M},$$

with initial value $u(0) = u_0 \in \mathcal{M}$. Using the orthogonal projection $P_u : L^2(\mathbb{R}^d) \to \mathcal{T}_u\mathcal{M}$ we can equivalently write

$$\mathrm{i}\varepsilon\partial_t u(t) = P_{u(t)}\big(H(t)u(t)\big), \quad u(0) = u_0 \in \mathcal{M}. \tag{2.5}$$

We note that (2.5) can also be stated in terms of the symplectic projection onto the tangent space, see C. Lubich's blue book [98, II.1.3].

Remark 2.3. In the time-independent and non-magnetic case, one can also treat initial values $\psi_0 \notin \mathcal{M}$ using continuous superpositions of thawed and frozen Gaussians, see [87, Ch. 5]. The extension of these to the case (2.1b), however, is beyond the scope of the present work.

For the manifold $\mathcal{M}$ defined in (2.4) the tangent space $\mathcal{T}_u\mathcal{M}$ takes the following simple form.

Lemma 2.4 ([87, Lemma 3.1])**.** *For $u \in \mathcal{M}$ we have*

$$\mathcal{T}_u\mathcal{M} = \{\varphi u \,|\, \varphi \text{ } d\text{-variate complex polynomial of degree at most } 2\}\,.$$

The approximation by Gaussian wave packets seems appropriate due to the following exactness result, which is a consequence of Lemma 2.4 together with (2.5) and Theorem 2.2.

Proposition 2.5 ([87, Prop. 3.2])**.** *Let $V(t,\cdot)$ be quadratic and $A(t,\cdot)$ be linear in space for all $t \in \mathbb{R}$. If $\psi_0 \in \mathcal{M}$, then the variational approximation u defined by (2.5) is exact, i.e., $u(t) = \psi(t)$, where ψ denotes the solution of (2.1a).*

We emphasize that in the situation of Proposition 2.5 the equations of motion (2.8) for the variational parameters (Theorem 2.6) simplify considerably. In particular, the expectation values become point evaluations and many terms vanish. Proposition 2.5 also includes the special case of linear magnetic vector potential and zero electrostatic potential, which is known for its dynamics with breathing oscillations, see e.g. [7, §VI].

In the next section we derive a system of ordinary differential equations to determine parameters of the variational solution $u \in \mathcal{M}$ and present error bounds for the variational approximation.

2.3 Main results

In the remaining paper we consider (2.1a) and (2.5) for initial data satisfying

$$\psi_0 = u_0 \in \mathcal{M} \quad \text{and} \quad \|u_0\|_{L^2} = 1. \tag{2.6}$$

Our first step is to derive equations of motions for the parameters defining the variational solution u. Then we show that in the limit $\varepsilon \to 0$, these equations tend to classical equations of motions. Moreover, we study geometric properties of the solution and the variational approximation. Finally, we state error bounds for the solution in the L^2-norm and for averages of observables. Our work generalizes the results in [87] in the sense that we treat time-dependent, magnetic Hamiltonians. We also generalize the results of [83, 114] from the position and momentum operator to sublinear observables in the sense of Assumption 2.1. For the sake of readability, we postpone the proofs to Sections 2.4 to 2.7.

2.3.1 Variational equations of motion

In order to write equations of motion for the parameters of a Gaussian wave packet $u \in \mathcal{M}$ we use the short notation

$$\begin{aligned} \mathcal{C}_\mathrm{R} &= \operatorname{Re}\mathcal{C}, & \mathcal{C}_\mathrm{I} &= \operatorname{Im}\mathcal{C}, \\ v &= (v_j)_{j=1}^d, & A &= (A_j)_{j=1}^d, \\ J_A &= \big(\partial_j A_k\big)_{j,k=1}^d, & (D^2_{A,v})_{k,l} &= \textstyle\sum_{j=1}^d \partial_l\partial_k A_j v_j. \end{aligned}$$

We start by deriving two equivalent sets of equations for $0 < \varepsilon \ll 1$. In the following section, we discuss the limit $\varepsilon \to 0$ and show that the two sets lead to the classical equations of motion for charged particles in a magnetic field given by the time-dependent Hamiltonian function

$$h(t, \widetilde{q}, \widetilde{p}) = \frac{1}{2}|\widetilde{p}|^2 - A(t, \widetilde{q}) \cdot \widetilde{p} + \widetilde{V}(t, \widetilde{q}), \quad (t, \widetilde{q}, \widetilde{p}) \in \mathbb{R} \times \mathbb{R}^{2d}, \tag{2.7}$$

cf. [58, 67]. The first set of equations of motion reads:

Theorem 2.6. *Let u_0 satisfy (2.6) and be given by its parameters $q_0, p_0, \mathcal{C}_0, \zeta_0$ defined in (2.4). Then, the parameters of the solution $u \in \mathcal{M}$ of (2.5) satisfy*

$$\dot{q} = p - \langle A \rangle_u, \tag{2.8a}$$

$$\dot{p} = \frac{\varepsilon}{2} \left\langle \nabla \mathrm{tr}\left(J_A^T \mathcal{C}_\mathrm{R} \mathcal{C}_\mathrm{I}^{-1} \right) \right\rangle_u + \langle J_A \rangle_u^T p - \langle \nabla \widetilde{V} \rangle_u, \tag{2.8b}$$

$$\begin{aligned} \dot{\mathcal{C}} = &-\mathcal{C}^2 + \langle D_{A,p}^2 \rangle_u + \langle J_A \rangle_u^T \mathcal{C} + \mathcal{C} \langle J_A \rangle_u - \langle \nabla^2 \widetilde{V} \rangle_u. \\ &+ \frac{\varepsilon}{2} \left\langle \nabla^2 \mathrm{tr}\left(J_A^T \mathcal{C}_\mathrm{R} \mathcal{C}_\mathrm{I}^{-1} \right) \right\rangle_u, \end{aligned} \tag{2.8c}$$

$$\begin{aligned} \dot{\zeta} = &\frac{1}{2}|p|^2 + \frac{\varepsilon}{2} \left\langle \mathrm{tr}\left(J_A^T \mathcal{C}_\mathrm{R} \mathcal{C}_\mathrm{I}^{-1} \right) \right\rangle_u + \frac{\mathrm{i}\varepsilon}{2} \mathrm{tr}(\mathcal{C}) \\ &- \frac{\varepsilon}{4} \mathrm{tr}\Big(\mathcal{C}_\mathrm{I}^{-1} \big(\frac{\varepsilon}{2} \left\langle \nabla^2 \mathrm{tr}\left(J_A^T \mathcal{C}_\mathrm{R} \mathcal{C}_\mathrm{I}^{-1} \right) \right\rangle_u + \langle J_A \rangle_u^T \mathcal{C}_\mathrm{R} + \mathcal{C}_\mathrm{R} \langle J_A \rangle_u + \langle D_{A,p}^2 \rangle_u \big) \Big) \\ &- \langle \widetilde{V} \rangle_u + \frac{\varepsilon}{4} \mathrm{tr}\big(\mathcal{C}_\mathrm{I}^{-1} \left\langle \nabla^2 \widetilde{V} \right\rangle_u \big), \end{aligned} \tag{2.8d}$$

with initial data $(q(0), p(0), \mathcal{C}(0), \zeta(0)) = (q_0, p_0, \mathcal{C}_0, \zeta_0)$.

The proof of Theorem 2.6 is given in Section 2.4. We observe that in terms of the classical Hamiltonian function h defined in (2.7), the equations of motion (2.8) can be rewritten as

$$\dot{q} = \langle \nabla_p h \rangle_u, \tag{2.9a}$$

$$\dot{p} = -\langle \nabla_q h \rangle_u, \tag{2.9b}$$

$$\dot{\mathcal{C}} = -\langle \nabla_{qq} h \rangle_u - \langle \nabla_{qp} h \rangle_u \mathcal{C} - \mathcal{C} \langle \nabla_{pq} h \rangle_u - \mathcal{C} \langle \nabla_{pp} h \rangle_u \mathcal{C}, \tag{2.9c}$$

$$\dot{\zeta} = -\langle h \rangle_u + \frac{\varepsilon}{4} \mathrm{tr}(B\, \mathcal{C}_\mathrm{I}^{-1}) + p^T \langle \nabla_p h \rangle_u. \tag{2.9d}$$

with the matrix $B \in \mathbb{C}^{d \times d}$ given by

$$B = \begin{pmatrix} \mathrm{Id}, \mathcal{C} \end{pmatrix} \langle \nabla^2 h \rangle_u \begin{pmatrix} \mathrm{Id} \\ \mathcal{C} \end{pmatrix}.$$

Later on, in Theorem 2.17 we extend these findings to the variational dynamics induced by a general a subquadratic Hamiltonian.

Remark 2.7. In order to solve (2.8) numerically, one might adapt the Boris algorithm originally proposed in [24] and recently analyzed in [62, 66]. This algorithm is constructed for the classical equations of motion for charged particle systems. Details or an efficient numerical algorithm are ongoing work which will be presented elsewhere. The averages appearing in the equations can be computed numerically by using Gauss-Hermite quadrature, cf. [87, Sec. 8]. In the special case of a linear potential A and quadratic potential V, the averages turn into point evaluations.

An alternative approach presented in [87] makes use of a factorization of the width matrix $\mathcal{C}$ due to Hagedorn. For the magnetic Schrödinger equation, it leads to differential equations for the factors of $\mathcal{C}$ instead of (2.8c). By [87, Lemma 3.16], we can write

$$\mathcal{C} = PQ^{-1} \quad \text{and} \quad \operatorname{Im}\mathcal{C} = (QQ^*)^{-1}, \tag{2.10}$$

with complex and invertible matrices P and Q. In addition, it holds $Y^T J Y = J$, where

$$Y \coloneqq \begin{pmatrix} \operatorname{Re} Q & \operatorname{Im} Q \\ \operatorname{Re} P & \operatorname{Im} P \end{pmatrix} \qquad \text{and} \qquad J \coloneqq \begin{pmatrix} 0 & -\mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix} \in \mathbb{R}^{2d\times 2d}, \tag{2.11}$$

i.e., Y is symplectic, or equivalently

$$Q^T P - P^T Q = 0, \tag{2.12a}$$

$$Q^* P - P^* Q = 2\mathrm{i}\,\mathrm{Id}. \tag{2.12b}$$

In fact, if Q and P are complex matrices satisfying (2.12), then Q and P are invertible and the matrix $\mathcal{C} = PQ^{-1}$ is symmetric with positive definite imaginary part $(QQ^*)^{-1}$. This allows us to write the Gaussian wave packet (2.4) as

$$u(\cdot, x) = \exp\Big(\frac{\mathrm{i}}{\varepsilon}\Big(\frac{1}{2}(x-q)^T PQ^{-1}(x-q) + p^T(x-q) + \zeta\Big)\Big) \tag{2.13}$$

and to derive equations of motion for the parameters (q, p, Q, P, ζ).

Corollary 2.8. *Let u_0 satisfy (2.6) and be given by the parameters q_0, p_0, $\mathcal{C}_0, \zeta_0$. Then the Gaussian wave packet (2.13) with parameters (q, p, Q, P, ζ) solving*

$$\dot{Q} = P - \langle J_A \rangle_u Q, \tag{2.14a}$$

$$\dot{P} = \langle J_A \rangle_u^T P + \frac{\varepsilon}{2}\big\langle \nabla^2 \operatorname{tr}\big(J_A \mathcal{C}_{\mathrm{R}} \mathcal{C}_{\mathrm{I}}^{-1}\big)\big\rangle_u Q + \big\langle D^2_{A,p}\big\rangle_u Q - \big\langle \nabla^2 \widetilde{V}\big\rangle_u Q, \tag{2.14b}$$

and (2.8a), (2.8b), and (2.8d) is the variational solution (2.5) with initial data

$$(q(0), p(0), \mathcal{C}(0), \zeta(0)) = (q_0, p_0, \mathcal{C}_0, \zeta_0).$$

If the initial matrices Q_0 and P_0 are symplectic, then $Q(t)$ and $P(t)$ are symplectic for all times $t \in \mathbb{R}$.

The proof of Corollary 2.8 is given in Section 2.4.

2.3.2 Equations of motion in the limit $\varepsilon \to 0$

The classical Hamiltonian function (2.7) induces the non-autonomous classical Hamiltonian system

$$\begin{aligned} \begin{pmatrix} \dot{\widetilde{q}}(t) \\ \dot{\widetilde{p}}(t) \end{pmatrix} &= J^{-1} \nabla h(t, \widetilde{q}(t), \widetilde{p}(t)) \\ &= \begin{pmatrix} \widetilde{p}(t) - A(t, \widetilde{q}(t)) \\ J_A^T(t, \widetilde{q}(t))\widetilde{p}(t) - \nabla \widetilde{V}(t, \widetilde{q}(t)) \end{pmatrix} \end{aligned} \tag{2.15}$$

with initial data $\widetilde{q}(s) = \widetilde{q}_s, \widetilde{p}(s) = \widetilde{p}_s$ and with J defined in (2.11). Since $A(t, \widetilde{q})$ and $\widetilde{V}(t, \widetilde{q})$ are sublinear and subquadratic with respect to $\widetilde{q}$, the right-hand side for the ordinary differential equation (2.15) is

locally Lipschitz continuous. There is no blow-up, since

$$\begin{aligned}\frac{1}{2}\partial_t\big(|\widetilde{q}|^2+|\widetilde{p}|^2\big) &= \widetilde{q}^T(\widetilde{p}-A(\widetilde{q}))+\widetilde{p}^T(J_A^T(\widetilde{q})\widetilde{p}-\nabla\widetilde{V}(\widetilde{q}))\\ &\leq C\big(1+|\widetilde{q}|^2+|\widetilde{p}|^2\big),\end{aligned}$$

where the constant $C>0$ depends on bounds of the potentials. By Gronwall's lemma, there is no finite time blow-up. This provides the existence of a unique global solution. The bound in [87, Lemma 3.15] states that $\langle\cdot\rangle_u$ tend to point evaluations at q as $\varepsilon\to 0$, i.e., $\langle A\rangle_u\to A(q)$. Hence, we observe that the magnetic equations of motion (2.8a) and (2.8b) tend to classical equations (2.15) as $\varepsilon\to 0$ and (2.8d) to

$$\dot{\zeta}=\frac{1}{2}|p|^2-\widetilde{V}(\cdot,q).$$

In order to link the set of equations (2.14) to classical mechanics, we consider the linearization of (2.15) along the position and momentum parameters (q,p), i.e.,

$$\begin{aligned}\begin{pmatrix}\dot{Q}\\ \dot{P}\end{pmatrix} &= J^{-1}\nabla^2 h(\cdot,\widetilde{q},\widetilde{p})\begin{pmatrix}Q\\ P\end{pmatrix}\\ &= \begin{pmatrix}P-J_A(\cdot,\widetilde{q})Q\\ \Big(D^2_{A(\cdot,\widetilde{q}),\widetilde{p}}-\nabla^2\widetilde{V}(\cdot,\widetilde{q})\Big)Q+J_A(\cdot,\widetilde{q})^TP\end{pmatrix}.\end{aligned}\tag{2.16}$$

By the same reasoning, we observe that the equations (2.14) tend to the linearized equations classical equations (2.16) as $\varepsilon\to 0$.

2.3.3 Averages

A further remarkable property of Gaussian wave packets is the conservation of several physical quantities. In the following, we recall the definitions of the linear and angular momentum for quantum dynamical systems.

Let $x=(x_1,\dots,x_N)$, where $x_k\in\mathbb{R}^3$, $k=1,\dots,N$ and $d=3N$, be position variables. We recall the follwoing definition given in [87, Chapter 3].

Definition 2.9. (a) The quantum mechanical total linear momentum operator is given by

$$\mathcal{P}:=-\mathrm{i}\varepsilon\sum_{k=1}^{N}\nabla_{x_k}.$$

(b) The quantum mechanical total angular momentum operator is given by

$$\mathcal{L}:=\sum_{k=1}^{N}x_k\times(-\mathrm{i}\varepsilon\nabla_{x_k})=-\mathrm{i}\varepsilon\sum_{k=1}^{N}\begin{pmatrix}x_{k_2}\partial_{k_3}-x_{k_3}\partial_{k_2}\\ x_{k_3}\partial_{k_1}-x_{k_1}\partial_{k_3}\\ x_{k_1}\partial_{k_2}-x_{k_2}\partial_{k_1}\end{pmatrix}.$$

Next, we state sufficient conditions on the potentials A and V, which lead to the conservation of averages of the observables from Definition 2.9.

Definition 2.10. We call a potential $W=(W_j)_{j=1,\dots,d}:(\mathbb{R}^3)^N\to\mathbb{R}^d$

(a) translation invariant, if

$$W_j(x_1,\dots,x_N) = W_j(x_1+r,\dots,x_N+r),$$

for all $r \in \mathbb{R}^3$ and $j = 1,\dots,d$,

(b) rotation invariant if for all orthogonal matrices $R \in \mathbb{R}^{3\times 3}$ with $\det R = 1$ it holds

$$W_j(x_1,\dots,x_N) = W_j(Rx_1,\dots,Rx_N),$$

where $j = 1,\dots,d$.

In the next lemma we provide a representation for the energy and state conservation properties of the momenta.

Lemma 2.11. *The following assertions hold.*

(a) We have $\|\psi(t)\|_{L^2} = \|u(t)\|_{L^2} = \|u_0\|_{L^2}$ *for all* $t \in \mathbb{R}$.

(b) If the potentials A *and* V *are both time-independent, then*

$$\langle H\rangle_{\psi(t)} = \langle H\rangle_{\psi_0} \quad \text{and} \quad \langle H\rangle_{u(t)} = \langle H\rangle_{u_0}.$$

(c) For $\varphi = \psi, u$ *the energy* $\langle H\rangle_\varphi$ *is given by*

$$\langle H(t)\rangle_{\varphi(t)} = \langle H(0)\rangle_{\varphi(0)} + \int_0^t \left\langle \mathrm{i}\varepsilon\partial_s A(s)\cdot\nabla\right\rangle_{\varphi(s)} + \left\langle \partial_s \widetilde{V}(s)\right\rangle_{\varphi(s)} \mathrm{d}s.$$

(d) For $\mathcal{P}$ *and* $\mathcal{L}$ *from Definition 2.9 we have:*

(i) If V *and* $A = (A_j)_{j=1}^d$ *given in Assumption 2.1 are invariant under translations*

$$\langle \mathcal{P}\rangle_{\psi(t)} = \langle \mathcal{P}\rangle_{\psi_0} \quad \text{and} \quad \langle \mathcal{P}\rangle_{u(t)} = \langle \mathcal{P}\rangle_{u_0}.$$

(ii) If $\widetilde{V}$ *defined in (2.2) is invariant under rotations and* $A(\cdot,x) = \alpha(\cdot)x$ *for some* $\alpha(\cdot) \in \mathbb{R}$, *then*

$$\langle \mathcal{L}\rangle_{\psi(t)} = \langle \mathcal{L}\rangle_{\psi_0} \quad \text{and} \quad \langle \mathcal{L}\rangle_{u(t)} = \langle \mathcal{L}\rangle_{u_0}.$$

The proof of Lemma 2.11 is given in Section 2.6.

2.3.4 L^2-error bound

In this section, we present the approximation property of the Gaussian wave packet with respect to the L^2-norm. Since our error bounds depend on parameters characterizing the Gaussian wave packet in (2.4), we first consider the boundedness of these parameters up to a fixed but arbitrary finite time $T > 0$ specified by ODE-theory.

Lemma 2.12. *For all times* $T > 0$, *the set of equations (2.8) is well-posed on* $[0,T]$ *independently of* ε. *Furthermore, the solution parameters are bounded independently of* ε, *i.e.*

$$|\nu| \le c_{\nu_0}, \qquad \text{for all } \nu \in \{q,p,\mathcal{C},\zeta\},$$

uniformly on $[0,T]$, *where* c_{ν_0} *depends on the parameters of the initial Gaussian* u_0, *on the potentials* V, A, *and on* T.

We note that by Corollary 2.8 the matrix $\mathcal{C}_\mathrm{I}$ is real symmetric, positive definite for all times t. To formulate the following results, we denote by $\rho > 0$ a lower bound on the smallest eigenvalue of $\mathcal{C}_\mathrm{I}$ on the finite time horizon $[0, T]$. For a discussion of relevant time scales on which ρ is sufficiently large compared to ε, called the Ehrenfest time, we refer to [87, Sec. 3.6]. With this, we can state our approximation result.

Theorem 2.13. *Let ψ, u be the solution of (2.1a) and (2.5), respectively, and let u_0 satisfy (2.6). Then the error bound*

$$\|\psi(t) - u(t)\|_{L^2} \leq tc\sqrt{\varepsilon}, \qquad t \in [0, T],$$

holds with a constant c which depends on ρ, the bounds on the parameters from Lemma 2.12 and on the potentials, but is independent of ε and t.

We provide the details and the proof of the theorem in Section 2.5.

2.3.5 Observable error bound

In classical mechanics physical states are described by the position and momentum parameters $\widetilde{q}, \widetilde{p} \in \mathbb{R}^d$. Observables are functions depending smoothly on $(\widetilde{q}, \widetilde{p}) \in \mathbb{R}^d \times \mathbb{R}^d$, see, for example, [67, 131]. Classical mechanics can be linked to quantum mechanics via Weyl quantization, which asigns a classical observable to a quantum mechanical one using semiclassical Fourier transformation, cf. [47, Thm. 4.14] or [67, 103]. Formally, for $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and an observable $\boldsymbol{a}$, we define

$$\mathrm{op}_\mathrm{Weyl}(\boldsymbol{a})\varphi(x) \coloneqq \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^{2d}} \boldsymbol{a}\Big(\frac{x+\widetilde{q}}{2}, \widetilde{p}\Big) \mathrm{e}^{\mathrm{i}\widetilde{p}\cdot(x-\widetilde{q})/\varepsilon} \varphi(\widetilde{q})\, \mathrm{d}(\widetilde{q}, \widetilde{p}).$$

The Weyl quantization of the projections to the first or second component of the classical variables are

$$\mathrm{op}_\mathrm{Weyl}(\widetilde{p})\varphi = -\mathrm{i}\varepsilon\nabla\varphi \quad \text{and} \quad \mathrm{op}_\mathrm{Weyl}(\widetilde{q})\varphi = x\varphi.$$

Further examples of physically relevant observables stemming from classical symbols are

$$\mathrm{op}_\mathrm{Weyl}(|\widetilde{p}|^2)\psi(x) = -\varepsilon^2\Delta\psi(x)$$

and, due to $\operatorname{div} A = 0$,

$$\begin{aligned}\mathrm{op}_\mathrm{Weyl}(A(\widetilde{q})\cdot\widetilde{p})\psi(x) &= \tfrac{1}{2}\left(A(x)\cdot(-\mathrm{i}\varepsilon\nabla) + (-\mathrm{i}\varepsilon\nabla)\cdot A(x)\right)\psi(x)\\ &= \left(A(x)\cdot(-\mathrm{i}\varepsilon\nabla)\right)\psi(x),\end{aligned}$$

and, of course,

$$\mathrm{op}_\mathrm{Weyl}(h(t))\psi(x) = H(t)\psi(x)$$

for the Hamiltonian function (2.7) and the magnetic Schrödinger operator (2.1b). An observable $\mathbf{A} = \mathrm{op}_\mathrm{Weyl}(\boldsymbol{a})$ defines for an L^2-normalised function $\varphi \in \mathcal{S}(\mathbb{R}^d)$ an expectation value,

$$\langle\varphi|\mathbf{A}\varphi\rangle = \int_{\mathbb{R}^d} \overline{\varphi(x)}(\mathbf{A}\varphi)(x)\mathrm{d}x,$$

and we investigate how expectation values issued by the variational approximation $u(t)$ differ from the ones of the true solution $\psi(t)$. For an error estimate relying on L^2 bounds, we have to restrict ourselves to sublinear classical observables.

Definition 2.14. The class of sublinear classical symbols is defined as smooth functions $\boldsymbol{a} : \mathbb{R}^{2d} \to \mathbb{R}$ such that for $\alpha \in \mathbb{N}_0^{2d}$ with $|\alpha| \geq 1$ there exists $C_\alpha > 0$

$$|\partial^\alpha \boldsymbol{a}(\widetilde{q}, \widetilde{p})| \leq C_\alpha$$

for all $(\widetilde{q}, \widetilde{p}) \in \mathbb{R}^d \times \mathbb{R}^d$.

For the expectation values of classical sublinear observables, we obtain the following error estimate that generalizes and improves the findings of N. King and T. Ohsawa [83, 114], where asymptotic accuracy of the order $\varepsilon^{3/2}$ has been observed and proved for the variational position and momentum expectation value.

Theorem 2.15. *Let ψ, u be the solution of (2.1a) and (2.5), respectively, and let u_0 satisfy (2.6). Moreover, let $\mathbf{A} = \mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})$ be an observable stemming from a classical sublinear observable $\boldsymbol{a}$ in the sense of Definition 2.14 such that $\boldsymbol{a} \circ \Phi^{t,s}$ is sublinear. Then we have the error bound*

$$\left|\langle \psi(t) | \mathbf{A}\psi(t)\rangle - \langle u(t) | \mathbf{A}u(t)\rangle\right| \leq t\, c\, \varepsilon^2,$$

for all $t \in [0, T]$. The error constant c depends on the parameter bounds of Lemma 2.12 for the time-interval $[0, T]$, in particular on the bounds for the width matrix $\mathcal{C}$, on the potentials, and on $\boldsymbol{a}$, but is independent of ε and t.

Note that the convergence in the observables is of order ε^2, while the convergence in the L^2-norm presented in Theorem 2.13 is of order $\sqrt{\varepsilon}$. This is an improvement of the results obtained in [87, Theorem 3.5], where $\mathcal{O}(\sqrt{\varepsilon})$ norm accuracy and an $\mathcal{O}(\varepsilon)$ estimate for the non-magnetic observable error were proved. The rest of the paper is devoted to the proofs of the equations of motion and the error estimates presented in this section.

2.4 Equations of motions: proof of Theorem 2.6 and corollary 2.8

In this section we derive equations of motion for the parameters $(q, p, \mathcal{C}, \zeta)$ as well as for the factorization matrices Q and P. To do so, we compute both sides of (2.5) and compare the coefficients.

Proof of Theorem 2.6. In order to use the formula for the orthogonal projection derived in [87, Prop. 3.14] for (2.5), we observe that derivatives with respect to x of a Gaussian wave packet turn into scalar functions of x times u. For notational simplicity, we omit the time-dependence and in the potentials A and V we omit the space variable x. In particular, we have

$$\mathrm{i}\varepsilon A \cdot \nabla u = -A \cdot \big(\mathcal{C}(x - q) + p\big)u, \tag{2.17a}$$

$$-\frac{\varepsilon^2}{2}\Delta u = \Big(\frac{1}{2}(x-q)^T\mathcal{C}^2(x-q) + p^T\mathcal{C}(x-q) + \frac{1}{2}|p|^2 - \frac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(\mathcal{C})\Big)u, \tag{2.17b}$$

and for the time derivative it holds that

$$\mathrm{i}\varepsilon\partial_t u(\cdot, x) = \Big(-\frac{1}{2}(x-q)^T\dot{\mathcal{C}}(x-q) + \dot{q}^T\mathcal{C}(x-q) - \dot{p}^T(x-q) + p^T\dot{q} - \dot{\zeta}\Big)u. \tag{2.18}$$

Motivated by the classical magnetic Hamiltonian system (2.15), we eliminate one degree of freedom by setting $\dot{q} = p - \langle A\rangle_u$, see [58, 67]. Incorporating the above formulas, we compare the coefficients in x on both sides of (2.5) and arrive at equations of motions of the form

$$\begin{aligned}
\dot{q} &= p - \langle A\rangle_u,\\
\dot{p} &= \big\langle J_A^T \mathcal{C}_{\mathrm{R}}(x-q)\big\rangle_u + \big\langle J_A\big\rangle_u^T p - \big\langle \nabla \widetilde{V}\big\rangle_u,\\
\dot{\mathcal{C}} &= -\mathcal{C}^2 + \big\langle D^2_{A,\mathcal{C}_{\mathrm{R}}(x-q)}\big\rangle_u + \big\langle D^2_{A,p}\big\rangle_u + \big\langle J_A\big\rangle_u^T \mathcal{C} + \mathcal{C}\big\langle J_A\big\rangle_u - \big\langle \nabla^2 \widetilde{V}\big\rangle_u,\\
\dot{\zeta} &= \frac{1}{2}|p|^2 + \big\langle A^T \mathcal{C}_{\mathrm{R}}(x-q)\big\rangle_u + \frac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(\mathcal{C})\\
&\quad - \frac{\varepsilon}{4}\mathrm{tr}\big(\mathcal{C}_{\mathrm{I}}^{-1}\big(\big\langle D^2_{A,\mathcal{C}_{\mathrm{R}}(x-q)}\big\rangle_u + \langle J_A\rangle_u^T \mathcal{C}_{\mathrm{R}} + \mathcal{C}_{\mathrm{R}}\langle J_A\rangle_u + \langle D^2_{A,p}\rangle_u\big)\big)\\
&\quad - \langle \widetilde{V}\rangle_u + \frac{\varepsilon}{4}\mathrm{tr}\big(\mathcal{C}_{\mathrm{I}}^{-1}\big\langle \nabla^2 \widetilde{V}\big\rangle_u\big).
\end{aligned}$$

It remains to extract the additional power of ε from the terms that contain the difference $x - q$. From

$$|u(x)|^2 = \exp\Big(-\frac{1}{\varepsilon}(x-q)^T \mathcal{C}_{\mathrm{I}}(x-q) - \frac{2}{\varepsilon}\mathrm{Im}\,\zeta\Big)$$

we obtain the derivative

$$\nabla|u(x)|^2 = -\frac{2}{\varepsilon}\mathcal{C}_{\mathrm{I}}(x-q)|u(x)|^2, \tag{2.19}$$

and apply integration by parts to obtain

$$\begin{aligned}
\big\langle A^T \mathcal{C}_{\mathrm{R}}(x-q)\big\rangle_u &= \big\langle A^T \mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\mathcal{C}_{\mathrm{I}}(x-q)\big\rangle_u\\
&= \int_{\mathbb{R}^d} A^T \mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\mathcal{C}_{\mathrm{I}}(x-q)|u(x)|^2 \mathrm{d}x\\
&= \frac{\varepsilon}{2}\big\langle \mathrm{tr}\,\big(J_A^T \mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\big)\big\rangle_u.
\end{aligned}$$

Similarly, we gain an order of ε for

$$\big(\big\langle J_A^T \mathcal{C}_{\mathrm{R}}(x-q)\big\rangle_u\big)_i = \big(\big\langle J_A^T \mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\mathcal{C}_{\mathrm{I}}(x-q)\big\rangle_u\big)_i = \frac{\varepsilon}{2}\big\langle \partial_i \mathrm{tr}\,\big(J_A^T \mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\big)\big\rangle_u,$$

as well as for

$$\begin{aligned}
\big(\big\langle D^2_{A,\mathcal{C}_{\mathrm{R}}(x-q)}\big\rangle_u\big)_{ij} &= \big(\big\langle D^2_{A,\mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}\mathcal{C}_{\mathrm{I}}^{-1}(x-q)}\big\rangle_u\big)_{ij}\\
&= \Big\langle \sum_{k,l,m=1}^{d} \partial_i\partial_j A_k \mathcal{C}_{\mathrm{R},kl}(\mathcal{C}_{\mathrm{I}}^{-1})_{lm} \sum_{n=1}^{d} \mathcal{C}_{\mathrm{I},mn}(x_n - q_n)\Big\rangle_u\\
&= \frac{\varepsilon}{2}\Big\langle \sum_{k,l,m=1}^{d} \partial_m\partial_i\partial_j A_k \mathcal{C}_{\mathrm{R},kl}(\mathcal{C}_{\mathrm{I}}^{-1})_{lm}\Big\rangle_u.
\end{aligned}$$

By the identity

$$\partial_{ij}\mathrm{tr}\,\big(J_A^T \mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\big) = \sum_{k,m,l=1}^{d} \partial_{ij}\partial_m A_k \mathcal{C}_{\mathrm{R},kl}(\mathcal{C}_{\mathrm{I}}^{-1})_{lm},$$

we conclude the equations of motion stated in (2.8). □

We now turn to the equations of motion for the Hagedorn factorization (2.10). The idea is to show that the product PQ^{-1} solves the same differential equation as $\mathcal{C}$ and conclude with the uniqueness of the variational solution u.

Proof of Corollary 2.8. We employ the differential identity

$$\partial_t(Q^{-1}) = -Q^{-1}\partial_t Q Q^{-1},$$

and the product rule to find that $\mathcal{C} = PQ^{-1}$ satisfies the differential equation

$$\dot{\mathcal{C}} = -PQ^{-1}\dot{Q}Q^{-1} + \dot{P}Q^{-1}$$

with $\partial_t Q = \dot{Q}$. Then, using (2.14), we see that this is the differential equation for $\mathcal{C}$ in (2.8c) and use (2.14) to find that $\mathcal{C} = PQ^{-1}$ satisfies the differential equation with $\partial_t Q = \dot{Q}$

$$\dot{\mathcal{C}} = -PQ^{-1}\dot{Q}Q^{-1} + \dot{P}Q^{-1}$$

$$\begin{aligned}
\dot{\mathcal{C}} &= P\partial_t(Q^{-1}) + \dot{P}Q^{-1} \\
&= -PQ^{-1}\left(P - \langle J_A\rangle_u Q\right)Q^{-1} \\
&\quad + \left(\left\langle D^2_{A,\mathcal{C}_{\mathrm{R}}(x-q)}\right\rangle_u Q + \left\langle D^2_{A,p}\right\rangle_u Q + \langle J_A\rangle_u^T P - \left\langle \nabla^2\widetilde{V}\right\rangle_u Q\right)Q^{-1} \\
&= -\mathcal{C}^2 + \mathcal{C}\langle J_A\rangle_u + \left\langle D^2_{A,\mathcal{C}_{\mathrm{R}}(x-q)}\right\rangle_u + \left\langle D^2_{A,p}\right\rangle_u + \langle J_A\rangle_u^T\mathcal{C} - \left\langle \nabla^2\widetilde{V}\right\rangle_u,
\end{aligned}$$

which are the differential equations for $\mathcal{C}$ in (2.8c).

Concerning the symplectic relation in (2.12), we have

$$\partial_t(Q^TP - P^TQ) = \dot{Q}^TP + Q^T\dot{P} - \dot{P}^TQ - P^T\dot{Q},$$

and by inserting the differential equations of P, Q given in (2.14),

$$\begin{aligned}
\dot{Q}^TP &= P^TP - Q^T\langle J_A\rangle_u^T P \\
Q^T\dot{P} &= Q^T\left(\left\langle D^2_{A,\mathcal{C}_{\mathrm{R}}(x-q)}\right\rangle_u + \left\langle D^2_{A,p}\right\rangle_u - \left\langle \nabla^2\widetilde{V}\right\rangle_u\right)Q + Q^T\langle J_A\rangle_u^T P \\
\dot{P}^TQ &= Q^T\left(\left\langle D^2_{A,\mathcal{C}_{\mathrm{R}}(x-q)}\right\rangle_u^T + \left\langle D^2_{A,p}\right\rangle_u^T - \left\langle \nabla^2\widetilde{V}\right\rangle_u^T\right)Q + P^T\langle J_A\rangle_u Q \\
P^T\dot{Q} &= P^TP - P^T\langle J_A\rangle_u Q,
\end{aligned}$$

we see that $Q^TP - P^TQ$ is constant. The same calculation holds for $\partial_t(Q^*P - P^*Q)$ with * replaced by ^{T}. Since p, q, A and V are real valued, we conclude

$$\partial_t(Q^*P - P^*Q) = \dot{Q}^*P + Q^*\dot{P} - \dot{P}^*Q - P^*\dot{Q} = 0,$$

which means that (2.12) holds true for all times. □

2.4.1 Equations of motion for a general Hamiltonian

The findings of Theorem 2.6 for the magnetic Schrödinger operator $H(t)$ extend to the dynamics for general Hamiltonian operators that are the Weyl quantization of a smooth function $h : \mathbb{R} \times \mathbb{R}^{2d} \to \mathbb{R}$ of subquadratic growth, that is, for all $\alpha \in \mathbb{N}_0^{2d}$ with $|\alpha| \geq 2$ there exists $C_\alpha > 0$ such that

$$|\partial^\alpha h(t, \widetilde{q}, \widetilde{p})| \leq C_\alpha \tag{2.20}$$

for all $t \in \mathbb{R}$ and $(\widetilde{q}, \widetilde{p}) \in \mathbb{R}^{2d}$. Note that the classical magnetic Hamiltonian function (2.7) is not subquadratic, but our analysis works for both cases.

A first step for the generalization is the construction of a suitable orthonormal basis of the tangent space of a Gaussian wave packet, which is done in [87, Lemma 3.12 and Theorem 4.1] for the non-magnetic case, where only the modulus squared of the wave packet matters. For convenience, we state the representation formulas of the basis functions that we use. Consider a Gaussian wave packet $u \in \mathcal{M}$ of unit norm, $\|u\| = 1$. The family $\{\varphi_n\}_{|n|\leq 2}$ with

$$\varphi_0 = u, \tag{2.21a}$$

$$\varphi_{e_j} = \sqrt{\frac{2}{\varepsilon}}\ \left(Q^{-1}(x-q)\right)_j\, u, \tag{2.21b}$$

$$\varphi_{e_j+e_k} = \frac{1}{\sqrt{\delta_{kj}+1}} \left(\frac{2}{\varepsilon}\ \left(Q^{-1}(x-q)\right)_j\ \left(Q^{-1}(x-q)\right)_k - (Q^*Q^{-T})_{j,k}\right) u, \tag{2.21c}$$

is an orthonormal basis of the tangent space $\mathcal{T}_u\mathcal{M}$ of $\mathcal{M}$ at u. For calculating the orthogonal projection to the tangent space, we make use of another representation via the raising and lowering operators $\mathcal{A}_j^\dagger$ and $\mathcal{A}_j$. These are the jth component of the vector-valued operators

$$\mathcal{A}^\dagger = \frac{\mathrm{i}}{\sqrt{2\varepsilon}} \left(P^* \mathrm{op}_{\mathrm{Weyl}}(\widetilde{q}-q) - Q^* \mathrm{op}_{\mathrm{Weyl}}(\widetilde{p}-p)\right),$$
$$\mathcal{A} = -\frac{\mathrm{i}}{\sqrt{2\varepsilon}} \left(P^T \mathrm{op}_{\mathrm{Weyl}}(\widetilde{q}-q) - Q^T \mathrm{op}_{\mathrm{Weyl}}(\widetilde{p}-p)\right),$$

respectively. Using the complete family of Hagedorn functions constructed by the infinite ladder process, we obtain that $\{\varphi_n\}_{|n|\leq 2}$ with

$$\varphi_0 = u, \quad \varphi_{e_j} = \mathcal{A}_j^\dagger u, \quad \varphi_{e_k+e_j} = \frac{1}{\sqrt{\delta_{kj}+1}}\ \mathcal{A}_j^\dagger\ \mathcal{A}_k^\dagger u, \tag{2.22}$$

see also [98, Chapter V.2] or [61, Theorem 3.3].

Equipped with the orthonormal basis (2.21) and (2.22), we can give an explicit formula for the quadratic polynomial generated by the orthogonal projection when acting on a general Hamiltonian operator.

Proposition 2.16 (Orthogonal projection)**.** *Let $h : \mathbb{R}^{2d} \to \mathbb{R}$ be smooth and of polynomial growth. Let $u \in \mathcal{M}$ be a Gaussian wave packet of unit norm, $\|u\| = 1$, with phase space center $z_0 = (q,p) \in \mathbb{R}^d \times \mathbb{R}^d$. Then,*

$$P_u(\mathrm{op}_{\mathrm{Weyl}}(h)u) = p_2 u,$$

where p_2 is the quadratic polynomial

$$p_2 : \mathbb{R}^d \to \mathbb{C},$$
$$p_2(x) = \beta + b^T(x-q) + \frac{1}{2}(x-q)^T B(x-q)$$

given by the complex coefficients

$$\beta = \langle h\rangle_u - \frac{\varepsilon}{4}\,\mathrm{tr}(B\ {\mathcal{C}_{\mathrm{I}}}^{-1}),$$
$$b = \begin{pmatrix}\mathrm{Id} & \mathcal{C}\end{pmatrix} \langle \nabla h\rangle_u \in \mathbb{C}^d,$$
$$B = \begin{pmatrix}\mathrm{Id} & \mathcal{C}\end{pmatrix} \langle \nabla^2 h\rangle_u \begin{pmatrix}\mathrm{Id} \\ \mathcal{C}\end{pmatrix} \in \mathbb{C}^{d\times d}.$$

The notation $\langle \boldsymbol{a}\rangle_u = \langle u \mid \mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})u\rangle$ refers to the expectation value of a quantized smooth observable $\boldsymbol{a} : \mathbb{R}^{2d} \to \mathbb{R}^L$ with respect to the Gaussian state u.

Proof. We use the Hagedorn wave packets $\{\varphi_n\}_{|n|\leq 2}$ associated with the Gaussian wave packet u as an orthonormal basis of the tangent space $\mathcal{T}_u\mathcal{M}$, see (2.21) and (2.22), and write the orthogonal projection as

$$P_u(\mathrm{op}_{\mathrm{Weyl}}(h)u) = \sum_{|n|\leq 2} \langle \varphi_n \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle \ \varphi_n.$$

Starting with the contribution for $n = 0$, we have

$$\langle \varphi_0 \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \langle u \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \langle h\rangle_u.$$

For the following, it will be useful to introduce the slim rectangular matrix $Z = (Q; P) \in \mathbb{C}^{2d\times d}$ with column vectors $Z_1, \dots, Z_d \in \mathbb{C}^{2d}$ and to write the ladder operators more compactly as

$$\mathcal{A}^\dagger = \frac{\mathrm{i}}{\sqrt{2\varepsilon}}\ Z^* J \mathrm{op}_{\mathrm{Weyl}}(\widetilde{z} - z), \qquad \mathcal{A} = -\frac{\mathrm{i}}{\sqrt{2\varepsilon}}\ Z^T J \mathrm{op}_{\mathrm{Weyl}}(\widetilde{z} - z).$$

For $n = e_j$ we have by (2.21), [87, Lemmas 4.1, and 4.2] that

$$\langle \varphi_{e_j} \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \langle u \mid \mathcal{A}_j \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \langle u \mid [\mathcal{A}_j, \mathrm{op}_{\mathrm{Weyl}}(h)]u\rangle.$$

Since the symbol of $\mathcal{A}_j$ is linear, we can use pseudodifferential calculus without remainders and obtain that the commutator satisfies

$$\begin{aligned}
[\mathcal{A}_j, \mathrm{op}_{\mathrm{Weyl}}(h)] &= -\frac{\mathrm{i}}{\sqrt{2\varepsilon}}\ \left[\mathrm{op}_{\mathrm{Weyl}}(Z_j^T J(\widetilde{z} - z)), \mathrm{op}_{\mathrm{Weyl}}(h)\right] \\
&= -\frac{\mathrm{i}}{\sqrt{2\varepsilon}} \frac{\varepsilon}{\mathrm{i}} \mathrm{op}_{\mathrm{Weyl}}(\{Z_j^T J(\widetilde{z} - z), h\}) \\
&= \sqrt{\frac{\varepsilon}{2}}\ \mathrm{op}_{\mathrm{Weyl}}(Z_j^T \nabla h),
\end{aligned} \tag{2.23}$$

where we have calculated the Poisson bracket according to

$$\{Z_j^T Jz, h\} = \nabla(Z_j^T Jz) \cdot J\nabla h = -Z_j^T \nabla h.$$

Therefore,

$$\langle \varphi_{e_j} \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \sqrt{\frac{\varepsilon}{2}} Z_j^T \langle \nabla h\rangle_u.$$

After summation, we therefore obtain that

$$\begin{aligned}
\sum_{j=1}^d \langle \varphi_{e_j} \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle\, \varphi_{e_j} &= \sum_{j=1}^d \langle \nabla h\rangle_u^T Z e_j e_j^T Q^{-1}(x - q)u \\
&= \langle \nabla h\rangle_u^T Z Q^{-1}(x - q)u \\
&= \langle \nabla h\rangle_u^T \begin{pmatrix} \mathrm{Id} \\ \mathcal{C} \end{pmatrix} (x - q)u,
\end{aligned}$$

which concludes the computation of the first order contributions. For the second order wave packets, we analogously compute the projection coefficient as

$$\begin{aligned}
\langle \varphi_{e_j+e_k} \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle &= \frac{1}{\sqrt{\delta_{kj}+1}} \langle \mathcal{A}_k^\dagger \mathcal{A}_j^\dagger u \mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle \\
&= \frac{1}{\sqrt{\delta_{kj}+1}} \langle \mathcal{A}_j^\dagger u \mid [\mathcal{A}_k, \mathrm{op}_{\mathrm{Weyl}}(h)]u\rangle \\
&= \frac{1}{\sqrt{\delta_{kj}+1}} \langle u \mid [\mathcal{A}_j, [\mathcal{A}_k, \mathrm{op}_{\mathrm{Weyl}}(h)]]u\rangle.
\end{aligned}$$

Using (2.23) twice, we obtain that the double commutator satisfies

$$\begin{aligned}\left[\mathcal{A}_j,[\mathcal{A}_k,\mathrm{op}_{\mathrm{Weyl}}(h)]\right] &= \sqrt{\frac{\varepsilon}{2}}\left[\mathcal{A}_j,\mathrm{op}_{\mathrm{Weyl}}(Z_k^T\nabla h)\right]\\ &= \frac{\varepsilon}{2}\,\mathrm{op}_{\mathrm{Weyl}}(Z_j^T\nabla(Z_k^T\nabla h))\\ &= \frac{\varepsilon}{2}\,\mathrm{op}_{\mathrm{Weyl}}(Z_j^T\nabla^2 h Z_k).\end{aligned}$$

This implies for the coefficient that

$$\langle\varphi_{e_j+e_k}\mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle = \frac{\varepsilon}{2\sqrt{\delta_{kj}+1}}\,Z_j^T\langle\nabla^2 h\rangle_u Z_k.$$

We now calculate the sum of all the second order contributions. We have

$$\begin{aligned}\sum_{|n|=2}\langle\varphi_n\mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle\varphi_n &= \sum_{j=1}^{d}\sum_{k=1}^{j}\langle\varphi_{e_j+e_k}\mid \mathrm{op}_{\mathrm{Weyl}}(h)u\rangle\varphi_{e_j+e_k}\\ &= \sum_{j,k=1}^{d}\frac{\varepsilon}{2\sqrt{2}}\,Z_j^T\langle\nabla^2 h\rangle_u Z_k\;\frac{1}{\sqrt{2}}\mathcal{A}_j^\dagger\mathcal{A}_k^\dagger u,\end{aligned}$$

where the complete summation over the full square of indices is compensated by a change in normalisation of the contributions for $j\neq k$. For the part of the sum that generates a constant prefactor for the Gaussian, we have

$$\begin{aligned}-\frac{\varepsilon}{4}\sum_{j,k=1}^{d}Z_j^T\langle\nabla^2 h\rangle_u Z_k\;(Q^*Q^{-T})_{j,k} &= -\frac{\varepsilon}{4}\mathrm{tr}(Q^*Q^{-T}Z^T\langle\nabla^2 h\rangle_u Z)\\ &= -\frac{\varepsilon}{4}\mathrm{tr}(\begin{pmatrix}\mathrm{Id} & \mathcal{C}\end{pmatrix}\langle\nabla^2 h\rangle_u\begin{pmatrix}\mathrm{Id}\\ \mathcal{C}\end{pmatrix}QQ^*).\end{aligned}$$

For the quadratic prefactor, we similarly obtain

$$\begin{aligned}&\frac{1}{2}\sum_{j,k=1}^{d}Z_j^T\langle\nabla^2 h\rangle_u Z_k\;\left(Q^{-1}(x-q)\right)_j\;\left(Q^{-1}(x-q)\right)_k\\ &= \frac{1}{2}(x-q)^T\begin{pmatrix}\mathrm{Id} & \mathcal{C}\end{pmatrix}\langle\nabla^2 h\rangle_u\begin{pmatrix}\mathrm{Id}\\ \mathcal{C}\end{pmatrix}(x-q).\end{aligned}$$

□

Let $h:\mathbb{R}\times\mathbb{R}^{2d}\to\mathbb{R}$ be continuous with respect to time $t\in\mathbb{R}$, and smooth, and of subquadratic growth in the sense of (2.20). Denote $H(t)=\mathrm{op}_{\mathrm{Weyl}}(h(t))$. Then, the time-dependent Schrödinger equation

$$i\varepsilon\partial_t\psi(t)=H(t)\psi(t),\quad \psi(0)=\psi_0$$

has a unique solution $\psi(t)=U(t,0)\psi_0$ for all times $t\in\mathbb{R}$ for all square integrable initial data $\psi_0\in L^2(\mathbb{R}^d)$, see [104] or [122, Def. 1]. The corresponding variational Gaussian wave packet obeys the following equations of motion.

Theorem 2.17 (Equations of motion for a general Hamiltonian)**.** *Let $u_0\in\mathcal{M}$ satisfy (2.6) and be given by its parameters $q_0,p_0,\mathcal{C}_0,\zeta_0$ defined in (2.4). Then, the parameters of the variational approximation*

$$\mathrm{i}\varepsilon\partial_t u(t)=P_{u(t)}(H(t)u(t)),\quad u(0)=u_0$$

satisfy the following set of ordinary differential equations (2.9) *subject to initial data* $(q(0), p(0), \mathcal{C}(0), \zeta(0)) = (q_0, p_0, \mathcal{C}_0, \zeta_0)$*, where* h *is now the given general subquadratic classical Hamiltonian function. The Hagedorn parameter matrices of the variational wave packet satisfy:*

$$\dot{P} = -\langle \nabla_{qq} h \rangle_u Q - \langle \nabla_{qp} h \rangle_u P, \qquad \dot{Q} = \langle \nabla_{pq} h \rangle_u Q + \langle \nabla_{pp} h \rangle_u P.$$

Moreover, the matrix factors Q*,* P *are symplectic, provided that the initial matrices* Q_0*,* P_0 *of the factorization* $\mathcal{C}_0 = P_0 Q_0^{-1}$ *are symplectic.*

Proof. We again use (2.18) and Proposition 2.16 and compare the coefficients with respect to the spatial variable x. We have one degree of freedom and set, inspired by (2.8a),

$$\dot{q} = \langle \nabla_p h \rangle_u.$$

Now, the claim follows by a direct calculation. □

The equations of motion given in Theorem 2.17 are indeed a generalization of the magnetic ones derived in Theorem 2.6 as we verify next.

Corollary 2.18. *In the special space of the magnetic Hamiltonian given in* (2.7) *we rediscover the equations of motion* (2.8)*. Moreover, if* $\varepsilon \to 0$ *and averages tend to point evaluations at the center point* q*, then the equations* (2.9a) *and* (2.9b) *tend to classical equations of motion for a general classical Hamiltonian function* h*.*

Proof. We have that

$$\langle \nabla_p h \rangle_u = p - \langle A \rangle_u, \quad \text{and} \quad -\langle \nabla_q h \rangle_u = -\mathrm{i}\varepsilon \langle J_A^T \nabla \rangle_u - \langle \nabla \widetilde{V} \rangle_u.$$

Furthermore, it is

$$\nabla^2 h(\cdot, q, p) = \begin{pmatrix} \nabla^2 \widetilde{V}(\cdot, q) - D^2_{A(\cdot,q),p} & -J_A^T \\ -J_A & \mathrm{Id} \end{pmatrix},$$

such that the trace part appearing in (2.9d) contains the terms

$$\begin{aligned} -\langle \nabla_{qq} h \rangle_u &= \langle D^2_{A,-\mathrm{i}\varepsilon\nabla} \rangle_u - \langle \nabla^2 \widetilde{V} \rangle_u, & -\langle \nabla_{qp} h \rangle_u \mathcal{C} &= \langle J_A^T \rangle_u \mathcal{C}, \\ -\mathcal{C} \langle \nabla_{pq} h \rangle_u &= \mathcal{C} \langle J_A \rangle_u, & -\mathcal{C} \langle \nabla_{pp} h \rangle_u \mathcal{C} &= -\mathcal{C}^2. \end{aligned}$$

For the scalar contribution of the projection Proposition 2.16 we observe by (2.17),

$$\begin{aligned} \langle h \rangle_u &= -\frac{\varepsilon^2}{2} \langle \Delta \rangle_u + \mathrm{i}\varepsilon \langle A \cdot \nabla \rangle_u + \langle \widetilde{V} \rangle_u \\ &= \frac{1}{2} |p|^2 + \frac{\varepsilon}{4} \mathrm{tr}\Big((\mathcal{C}_\mathrm{R}{}^2 + \mathcal{C}_\mathrm{I}{}^2) \mathcal{C}_\mathrm{I}^{-1} \Big) - \langle A^T \big((\mathcal{C}_\mathrm{R} + \mathrm{i}\mathcal{C}_\mathrm{I})((x-q)+p) \big) \rangle_u + \langle \widetilde{V} \rangle_u \\ &= \frac{1}{2} |p|^2 + \frac{\varepsilon}{4} \mathrm{tr}\Big((\mathcal{C}_\mathrm{R}{}^2 + \mathcal{C}_\mathrm{I}{}^2) \mathcal{C}_\mathrm{I}^{-1} \Big) - \langle A^T \big(\mathcal{C}_\mathrm{R}(x-q) + p \big) \rangle_u + \langle \widetilde{V} \rangle_u. \end{aligned}$$

Finally, we calculate the following trace, appearing in (2.9d), as

$$\begin{aligned} -\mathrm{tr}\Big((\mathcal{C}_\mathrm{R}{}^2 + \mathcal{C}_\mathrm{I}{}^2) \mathcal{C}_\mathrm{I}^{-1} \Big) + \mathrm{tr}\Big(\mathcal{C}^2 \mathcal{C}_\mathrm{I}^{-1} \Big) &= \mathrm{tr}\Big((\mathcal{C}_\mathrm{R}{}^2 - \mathcal{C}_\mathrm{I}{}^2 + \mathrm{i}(\mathcal{C}_\mathrm{I}\mathcal{C}_\mathrm{R} + \mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I})) \mathcal{C}_\mathrm{I}^{-1} \Big) \\ &= -2 \,\mathrm{tr}(\mathcal{C}_\mathrm{I}) + 2\mathrm{i} \,\mathrm{tr}(\mathcal{C}_\mathrm{R}) \\ &= 2\mathrm{i} \,\mathrm{tr}(\mathcal{C}), \end{aligned}$$

such that, together with

$$p^T\langle\nabla_p h\rangle_u = |p|^2 - p^T\langle A\rangle_u,$$

we obtain the differential equation (2.8d). □

2.5 L^2-error bound: proof of Lemma 2.12 and Theorem 2.13

This section is devoted to the wellposedness of the equations of motion (2.8) and the approximation quality of the variational solution in the L^2-norm.

We first state the following lemma which will be used frequently to obtain error bound with respect to ε. We recall that the lower bound on the eigenvalues of $\mathcal{C}_\mathrm{I}$ was denoted by $\rho > 0$.

Lemma 2.19 ([87, Lemma 3.8]). *For any $m \geq 0$ there exists a constant c_m such that for all $\varepsilon > 0$ it holds*

$$(\pi\varepsilon)^{-\frac{d}{4}} \det(\mathcal{C}_\mathrm{I})^{\frac{1}{4}} \Big(\int |x|^{2m} \exp\big(-\frac{1}{\varepsilon} x^T \mathcal{C}_\mathrm{I} x \big)\, \mathrm{d}x \Big)^{\frac{1}{2}} \leq c_m \Big(\frac{\varepsilon}{\rho}\Big)^{\frac{m}{2}},$$

where c_m is independent of ε and ρ.

We now prove the wellposedness result for (2.8) and show the boundedness of the parameters solving (2.8).

Proof of Lemma 2.12. We show that the right-hand side of (2.8) satisfies a local Lipschitz condition with Lipschitz constant independent of ε. To this end it is sufficient if the derivatives with respect to parameters $q, p, \mathcal{C}_\mathrm{R}, \mathcal{C}_\mathrm{I}, \zeta$ are bounded on a bounded domain. Then, we obtain a local solution and, as in Section 2.3.2, we can show that there is no blow-up.

The potentials in the averages of the equations of motion in (2.8) do not depend on ε. However, we need to carefully treat the absolute values of the Gaussian wave packet, since they contain ε in the denominator. By the chain rule, it is sufficient to first calculate the derivatives of averages of some arbitrary potential $\widehat{U}$, which is independent of the parameters. Then, the average has the form

$$\langle\widehat{U}\rangle_u = \frac{\sqrt{\det(\mathcal{C}_\mathrm{I})}}{(\pi\varepsilon)^{\frac{d}{2}}} \int \widehat{U}(x) \exp\left(-\frac{1}{\varepsilon}(x-q)^T \mathcal{C}_\mathrm{I}(x-q) \right) \mathrm{d}x,$$

from which we see that, in this case, the average only depends on q and $\mathcal{C}_\mathrm{I}$. Let u be a Gaussian wave packet with $\|u\|_{L^2} = 1$. By (2.19) we obtain

$$\begin{aligned}
&\frac{\sqrt{\det(\mathcal{C}_\mathrm{I})}}{(\pi\varepsilon)^{\frac{d}{2}}}\, \partial_q \exp\left(-\frac{1}{\varepsilon}(x-q)^T \mathcal{C}_\mathrm{I}(x-q) \right) \\
&= \frac{\sqrt{\det(\mathcal{C}_\mathrm{I})}}{(\pi\varepsilon)^{\frac{d}{2}}}\, \frac{2}{\varepsilon}\mathcal{C}_\mathrm{I}(x-q) \exp\left(-\frac{1}{\varepsilon}(x-q)^T \mathcal{C}_\mathrm{I}(x-q) \right) \\
&= -\nabla |u(x)|^2,
\end{aligned}$$

thus, using integration by parts, the derivative of the average with respect to to q is given by

$$\partial_q \langle\widehat{U}(x)\rangle_u = \langle\nabla\widehat{U}(x)\rangle_u.$$

We continue with derivatives with respect to $\mathcal{C}_\mathrm{I}$. For a differentiable matrix function $F : \mathbb{R}^{d\times d} \to \mathbb{R}$ and a general invertible, symmetric matrix $M = (m_{ij})_{i,j=1,\dots,d}$ we define the componentwise derivation matrix

$$\partial_M F(M) \coloneqq (\partial_{m_{ij}} F(M))_{i,j=1,\dots,d} \in \mathbb{R}^{d\times d}.$$

By [78, Part 0.8.10] we have

$$\partial_M a^T M b = ab^T \quad \text{and} \quad \partial_M \det(M) = \det(M) M^{-1}$$

and consequently,

$$\partial_M \sqrt{\det(M)} = \frac{1}{2}\sqrt{\det(M)} M^{-1}.$$

Hence, it follows that

$$\partial_{\mathcal{C}_\mathrm{I}} \exp\left(-\frac{1}{\varepsilon}(x-q)^T \mathcal{C}_\mathrm{I}(x-q)\right) = -\frac{1}{\varepsilon}(x-q)(x-q)^T \exp\left(-\frac{1}{\varepsilon}(x-q)^T \mathcal{C}_\mathrm{I}(x-q)\right)$$

and

$$\partial_{\mathcal{C}_\mathrm{I}} \langle \widehat{U}(x)\rangle_u = -\frac{1}{\varepsilon}\left\langle (x-q)(x-q)^T \widehat{U}(x)\right\rangle_u + \frac{1}{2} I^{-1} \left\langle \widehat{U}(x)\right\rangle_u.$$

By Lemma 2.19 we have $\left|\left\langle (x-q)(x-q)^T \widehat{U}(x)\right\rangle_u\right| \leq C\varepsilon$ for parameters on a bounded domain.

For potentials depending on the parameters, we use again that we are on a bounded domain and that the dependence on ε of the potentials in (2.8) is such that ε does not enter the denominator. □

We now turn to the L^2-error bound and adapt the proof of [87, Theorem 3.5] to the magnetic case and note that the multiplication potential $\widetilde{V}$ is already covered. In order to demonstrate the dependence of the constant in the error bound, we carry out the proof for the advection term.

Proof of Theorem 2.13. From the proof of [87, Theorem 3.5] we know that

$$\left\|\psi(t) - u(t)\right\|_{L^2} \leq \int_0^t \frac{1}{\varepsilon} \left\|Hu - P_u(Hu)\right\|_{L^2} \mathrm{d}s.$$

(a) We write the action of the magnetic Schrödinger operator H on a Gaussian u with width $\mathcal{C}$ and phase space center (q,p) as

$$Hu = -\frac{\varepsilon^2}{2}\Delta u + Yu + \widetilde{V}u$$

with

$$Y_u \coloneqq -A \cdot (\mathcal{C}(x-q) + p). \tag{2.25}$$

We perform a second order Taylor expansion of the potentials Y_u and $\widetilde{V}$ around the point q and denote by W_q and $\widetilde{W}_q$ the respective remainders. Then,

$$(\mathrm{Id} - P_u)(Hu) = (\mathrm{Id} - P_u)(W_q u + \widetilde{W}_q u)$$

and

$$\left\|\psi(t) - u(t)\right\|_{L^2} \leq \int_0^t \frac{1}{\varepsilon} \left\|W_q u + \widetilde{W}_q u\right\|_{L^2} \mathrm{d}s.$$

Since

$$W_q = \frac{1}{2}\sum_{|\alpha|=3}(x-q)^\alpha \int_0^1 (1-\theta)^2 \partial^\alpha Y_u\big(q+\theta(x-q)\big)\mathrm{d}\theta,$$

we bound $\big\|W_q u\big\|_{L^2}$ by finding a bound on $\partial^\alpha Y_u\big(q+\theta(x-q)\big)$, which then leads us to

$$|W_q(x)|^2 \leq C|x-q|^6.$$

By norm conservation and Lemma 2.19 the claim that $\big\|W_q u\big\|_{L^2} = \mathcal{O}(\varepsilon^{3/2})$ follows. For the third derivative of $\partial_{lmn} Y_u$ where $l,m,n = 1,\dots,d$, we have

$$\begin{aligned}\partial_{lmn} Y_u = (\partial_{lmn}A)^T\mathcal{C}(x-q) + (\partial_{lmn}A)^T p \\ + \big((\partial_{lm}A)^T\mathcal{C}\big)_n + \big((\partial_{ln}A)^T\mathcal{C}\big)_m + \big((\partial_{mn}A)^T\mathcal{C}\big)_l,\end{aligned} \tag{2.26}$$

where $\partial_{lmn}A$ is meant component wise. The term $x-q$ in (2.26) evaluated at $x = q+\theta(x-q)$ has the form

$$\theta(\partial_{lmn}A)^T\mathcal{C}(x-q).$$

By Lemma 2.19 we gain additional orders of ε, and we thus neglect the first summand in (2.26). The remaining terms are bounded again using Lemma 2.19.

(b) In the general subquadratic case, we use that the action of a semiclassical pseudodifferential operator on a Gaussian wave packet can be approximated by a polynomial prefactor, see [122, Lemma 14 in §2.3]. For any $\ell \in \mathbb{N}$ there exists a polynomial $\mathcal{Q}_\ell$ of degree ℓ, such that

$$Hu = \mathcal{Q}_\ell\, u + \mathcal{O}(\varepsilon^{(\ell+1)/2}),$$

i.e., we have

$$Hu - P_u(Hu) = W_{u,\ell}\, u + \mathcal{O}(\varepsilon^{(\ell+1)/2}), \tag{2.27}$$

with a remainder potential $W_{u,\ell}$. We now fix $\ell = 2$ and denote the corresponding cubic remainder potential $W_u = W_{u,2}$. The proof then works along the lines of the magnetic case. □

2.6 Expectation values: proof of Lemma 2.11

In this section we adapt the proofs of [87, Section 3.2] on conservation properties to the time-dependent, magnetic case. Due to time-dependence, the energy will not be a conserved quantity.

Let ψ be the exact solution of (2.1a) and u the variational solution (2.5) such that (2.6) holds.

Proof of Lemma 2.11. The proof of norm conservation and the energy formula can be done in the same way as in [87]. We only show the conservation of total linear and angular momentum.

By [98, Theorem 1.3] or [48, Lemma 4.1] it is sufficient to show that $H(t)$ commutes with P and L, respectively, for each $t \in [0,T]$. By [87] it follows that $\mathcal{P}A_{k_j} = 0$ for all $k \in \{1,\dots,N\}$ and $j \in \{1,2,3\}$. We further calculate

$$\mathcal{P}(A\cdot\nabla)\psi = \sum_{k=1}^{N}\sum_{j=1}^{3}(\mathcal{P}A_{k_j})\partial_{k_j}\psi + A_{k_j}\mathcal{P}\partial_{k_j}\psi = (A\cdot\nabla)\mathcal{P}\psi.$$

Furthermore, a tedious calculation shows that $(A \cdot \nabla)\mathcal{L}\psi = \mathcal{L}(A \cdot \nabla)\psi$ if and only if

$$\sum_{l=1}^{N} \begin{pmatrix} A_{l_2}\partial_{l_3} - A_{l_3}\partial_{l_2} \\ A_{l_3}\partial_{l_1} - A_{l_1}\partial_{l_3} \\ A_{l_1}\partial_{l_2} - A_{l_2}\partial_{l_1} \end{pmatrix} \psi = \sum_{k=1}^{N}\sum_{j=1}^{3}\sum_{l=1}^{N} \begin{pmatrix} x_{l_2}(\partial_{l_3}A_{k_j})\partial_{k_j} - x_{l_3}(\partial_{l_2}A_{k_j})\partial_{k_j} \\ x_{l_3}(\partial_{l_1}A_{k_j})\partial_{k_j} - x_{l_1}(\partial_{l_3}A_{k_j})\partial_{k_j} \\ x_{l_1}(\partial_{l_2}A_{k_j})\partial_{k_j} - x_{l_2}(\partial_{l_1}A_{k_j})\partial_{k_j} \end{pmatrix} \psi$$

holds true. This condition is fulfilled if

$$\partial_{l_m} A_{k_j} = \alpha \delta_{l_m,k_j} \quad \text{und} \quad A_{l_n} = \alpha x_{l_n}$$

holds true for some $\alpha \in \mathbb{R}$, $j, n, m \in \{1, 2, 3\}$, and $k, l \in \{1, \dots, N\}$ and thus, if $A(\cdot, x) = \alpha(\cdot)x$ holds. □

2.7 Error bound for averages of observables: proof of Theorem 2.15

In this section we give the proof of Theorem 2.15. We proceed in three steps: First, we follow [87, Section 6.7] and establish an integral representation for the error that involves a commutator with the time-evolved observable. Second, we prove Egorov's theorem for the time-evolution of observables in the general context of magnetic Schrödinger operators. Third, we derive a semiclassical expansion of averages with respect to Gaussian wave packets. The combination of these steps then allows us to prove Theorem 2.15. We note that the semiclassical expansion of the averages is crucial for improving the observable estimate in [87, Theorem 3.5]. This section applies for both the magnetic and the general subquadratic hamiltonian case. For better readability, some arguments will be provided for the magnetic case only, but with natural slight modifications they also apply for the general subquadratic case.

2.7.1 Error representation

We start with a useful a posteriori representation for the observable error. To this end, let $U(t, s)$ be the evolution family given by Theorem 2.2 and $\mathbf{A}$ an observable. We introduce the notation

$$\widetilde{\mathbf{A}}(t, s) := U(s, t)\mathbf{A}U(t, s), \qquad t, s \in \mathbb{R}.$$

Lemma 2.20. *Let ψ be the solution of (2.1a) and u the solution of (2.5). If the initial value $\psi_0 = u_0 \in \mathcal{M}$ is a Gaussian wave packet with $\|u_0\|_{L^2} = 1$, then the error of the observables takes the form*

$$\begin{aligned} &\langle \psi(t)|\mathbf{A}\psi(t)\rangle - \langle u(t)|\mathbf{A}u(t)\rangle \\ &= \int_0^t \frac{1}{\mathrm{i}\varepsilon}\langle u(s)\Big| \left(\overline{W}_{u(s)}\widetilde{\mathbf{A}}(t, s) - \widetilde{\mathbf{A}}(t, s)W_{u(s)}\right) u(s)\rangle \,\mathrm{d}s, \end{aligned} \tag{2.28}$$

where the remainder potential $W_u : \mathbb{R}^d \to \mathbb{C}$ depends on the Gaussian wave packet u. In the general subquadratic case, it has been previously defined in (2.27). In the magnetic Schrödinger case, it satisfies

$$\begin{aligned} W_u = X_u(q) - \langle X_u\rangle_u + \frac{\varepsilon}{4}\mathrm{tr}(\mathcal{C}_{\mathrm{I}}{}^{-1}\langle \nabla^2 X_u\rangle_u) + (\nabla X_u(q) - \langle \nabla X_u\rangle_u)^T (x - q) \\ + \frac{1}{2}(x - q)^T \left(\nabla^2 X_u(q) - \langle \nabla^2 X_u\rangle_u\right)(x - q) + R(X_u), \end{aligned} \tag{2.29}$$

with $X_u = Y_u + \widetilde{V}$ defined in (2.25) and (2.2), respectively, and $R(X_u)$ being the remainder potential of the quadratic Taylor expansion of X_u around the point q. For the non-magnetic Schrödinger case $A = 0$, we have $Y_u = 0$ and $W_u : \mathbb{R}^d \to \mathbb{R}$.

Proof. Let $U(t,s)$ be the evolution family, such that the exact solution of (2.1a) is given by (2.3). Using $\psi_0 = u_0$ and $U(t,t) = \mathrm{Id}$ we calculate

$$\begin{aligned}
&\langle u(t)|\mathbf{A}u(t)\rangle - \langle \psi(t)|\mathbf{A}\psi(t)\rangle \\
&\qquad = \langle u(t)|U(t,t)\mathbf{A}U(t,t)u(t)\rangle - \langle U(t,0)u(0)|\mathbf{A}U(t,0)u(0)\rangle \\
&\qquad = \langle u(t)|U(t,t)\mathbf{A}U(t,t)u(t)\rangle - \langle u(0)|U(0,t)\mathbf{A}U(t,0)u(0)\rangle \\
&\qquad = \int_0^t \frac{\partial}{\partial s}\langle u(s)|\underbrace{U(s,t)\mathbf{A}U(t,s)}_{=\widetilde{\mathbf{A}}(t,s)}u(s)\rangle\,\mathrm{d}s.
\end{aligned}$$

Employing the differential properties of the evolution family, that is, $\mathrm{i}\varepsilon\partial_t U(t,s) = H(t)U(t,s)$ and $-\mathrm{i}\varepsilon\partial_t U(s,t) = U(s,t)H(t)$, we obtain

$$\begin{aligned}
\frac{\partial}{\partial s}\widetilde{\mathbf{A}}(t,s) &= \frac{1}{\mathrm{i}\varepsilon}\big(H(s)U(s,t)\mathbf{A}U(t,s) - U(s,t)\mathbf{A}U(t,s)H(s)\big) \\
&= \frac{1}{\mathrm{i}\varepsilon}\big(H(s)\widetilde{\mathbf{A}}(t,s) - \widetilde{\mathbf{A}}(t,s)H(s)\big).
\end{aligned} \tag{2.30}$$

Since the variational evolution satisfies $\mathrm{i}\varepsilon\partial_t u(t) = P_{u(t)}H(t)u(t)$, we then have

$$\begin{aligned}
\frac{\partial}{\partial s}\langle u(s)|\widetilde{\mathbf{A}}(t,s)u(s)\rangle = \frac{1}{\mathrm{i}\varepsilon}\Big(&\langle(\mathrm{Id}-P_{u(s)})H(s)u(s)|\widetilde{\mathbf{A}}(t,s)u(s)\rangle\Big) \\
&-\langle u(s)|\widetilde{\mathbf{A}}(t,s)(\mathrm{Id}-P_{u(s)})H(s)u(s)\rangle\Big).
\end{aligned}$$

We arrive at (2.28), using that

$$(\mathrm{Id}-P_{u(s)})H(s)u(s) = X_{u(s)}u(s) - P_{u(s)}(X_{u(s)}u(s)) = W_{u(s)}u(s).$$

The claimed form of the remainder potential $W_{u(s)} : \mathbb{R}^d \to \mathbb{C}$ follows from [87, Proposition 3.14], since the proof of the projection formula there also applies for the potential function $X_{u(s)}$ even though it is complex-valued. □

2.7.2 Egorov's theorem

Further, to prove Theorem 2.15 we have to establish a variant of Egorov's theorem, which connects the time-evolved quantum observable $\widetilde{\mathbf{A}}(t,s)$, in case it originates from a Weyl-quantized $\mathbf{A} = \mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})$, with the evolution map of the classical Hamiltonian system. Recall that since A and $\widetilde{V}$ are sublinear and subquadratic, respectively, we obtain a unique global solution to the ordinary differential equation (2.15). We denote by

$$\Phi^{t,s} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}, \quad (\widetilde{q}_s, \widetilde{p}_s) \mapsto (\widetilde{q}_s(t), \widetilde{p}_s(t))$$

the classical propagator, which maps initial values at time s to the solution of (2.15) at time t. For any $\widetilde{z} = (\widetilde{q}, \widetilde{p})$, it satisfies the evolution equation

$$\begin{aligned}
\partial_t \Phi^{t,s}(\widetilde{z}) &= -J(\nabla_{\widetilde{z}} h)(t, \Phi^{t,s}(\widetilde{z})), \\
\Phi^{s,s}(\widetilde{z}) &= \widetilde{z}.
\end{aligned} \tag{2.31}$$

Both in the magnetic and the general subquadratic case, the classical propagator $\Phi^{t,\tau}$ is a diffeomorphism with inverse $(\Phi^{t,\tau})^{-1} = \Phi^{\tau,t}$. For time-independent, subquadratic Hamiltonians it is well-established that

$$\widetilde{\mathbf{A}}(t,0) = \mathrm{op}_{\mathrm{Weyl}}\left(\boldsymbol{a} \circ \Phi^{t,0}\right) + \mathcal{O}(\varepsilon^2).$$

However, to the best of our knowledge, in the literature a proof of the Egorov approximation for the non-autonomous case is not available, and the proofs presented for example in [25], [137, Chapter 11], or [122, Thm. 12] assume time-independent or compactly supported Hamiltonians and thus do not cover our more general situation. The main difficulties are the time-dependence of the Hamiltonian operator $H(t)$, which prevents energy conservation, and the allowed sublinear growth of the observables.

Proposition 2.21 (time-dependent Egorov–theorem)**.** *Let $\mathbf{A} = \mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})$ be a quantum observable stemming from a smooth, sublinear classical observable $\boldsymbol{a}$ in the sense of Definition 2.14. Further, let $\widetilde{\boldsymbol{a}} : \mathbb{R} \times \mathbb{R} \times \mathbb{R}^{2d} \to \mathbb{R}$, $(t, s, \widetilde{z}) \mapsto \widetilde{\boldsymbol{a}}(t, s, \widetilde{z})$ be defined by*

$$\widetilde{\boldsymbol{a}}(t, s, \widetilde{z}) = \boldsymbol{a} \circ \Phi^{t,s}(\widetilde{z}). \tag{2.32}$$

We consider two cases.

(a) *The Hamiltonian operator stems from a classical, subquadratic function h. Then, the observable given in (2.32) is sublinear and for all $\varphi \in L^2(\mathbb{R}^d)$ we have*

$$\left\| \left(\widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}(t,s)\right)\right)\varphi \right\|_{L^2} \leq C\,\varepsilon^2\,\mathrm{e}^{C|t-s|}\,\|\varphi\|_{L^2}$$

for all $s, t \in \mathbb{R}$.

(b) *The Hamiltonian operator is a magnetic Schrödinger operator. We assume that the observable given in (2.32) is of time-exponential growth in the following sense. There exists a smooth nonnegative function $\Gamma(t,s) \geq 0$ such that for any $\alpha \in \mathbb{N}^{2d}$ there exists $C_\alpha > 0$ with*

$$|\partial_{\widetilde{z}}^{\alpha} \widetilde{\boldsymbol{a}}(t, s, \widetilde{z})| \leq C_{\boldsymbol{a},\alpha}\ \exp(|\alpha|\,\Gamma(t,s))$$

for all $\widetilde{z} \in \mathbb{R}^{2d}$ and all $t, s \in \mathbb{R}$. Then, for any $\varphi \in L^2(\mathbb{R}^d)$ such that $\mathrm{op}_{\mathrm{Weyl}}(\widetilde{z})\varphi \in L^2(\mathbb{R}^d)$, we then have

$$\left\| \left(\widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}(t,s)\right)\right)\varphi \right\|_{L^2} \leq C\,\varepsilon^2\,\mathrm{e}^{C|t-s|}\,\left\|\mathrm{op}_{\mathrm{Weyl}}(\widetilde{z})\varphi\right\|_{L^2},$$

for all $s, t \in \mathbb{R}$.

The constant $C > 0$ depends on derivative bounds of the potentials A, V and the observable $\boldsymbol{a}$, but not on ε, t, s. In particular, $C = 0$ for A linear and V quadratic.

Proof. (1) We start by discussing the growth of the function $\widetilde{\boldsymbol{a}}(t, s, \widetilde{z})$ for case (a). For first order derivatives with respect to $(\widetilde{q}, \widetilde{p})$ of the classical propagator we have

$$D\Phi^{t,s} = \mathrm{Id} + J^{-1} \int_s^t \nabla^2 h(\tau, \Phi^{\tau,s})\, D\Phi^{\tau,s}\,\mathrm{d}\tau,$$

and thus

$$\left\|D\Phi^{t,s}\right\|_{\infty} \leq 1 + \int_s^t \sup_{\widetilde{z} \in \mathbb{R}^{2d}} \|\nabla_{\widetilde{z}}^2 h(\tau, \widetilde{z})\|\, \|D\Phi^{\tau,s}\|_{\infty}\,\mathrm{d}\tau.$$

Since the Hamiltonian function $h(t,\cdot)$ is subquadratic, we have

$$\Gamma(t,s) := \int_s^t \sup_{\widetilde{z}\in\mathbb{R}^{2d}} \|\nabla_{\widetilde{z}}^2 h(\tau,\widetilde{z})\| \mathrm{d}\tau < \infty,$$

and by Gronwall's lemma

$$\left\|D\Phi^{t,s}\right\|_\infty \leq \exp(\Gamma(t,s)).$$

Moreover, for any $\alpha\in\mathbb{N}^{2d}$ with $|\alpha|\geq 1$ there exists a constant $C_\alpha>0$ such that

$$|\partial_{\widetilde{z}}^\alpha \Phi^{t,s}(\widetilde{z})| \leq C_\alpha \exp(|\alpha|\,\Gamma(t,s))$$

for all $t,s\in\mathbb{R}$ and all $\widetilde{z}\in\mathbb{R}^{2d}$, see [25, Lemma 2.2] for a proof that literally applies to the non-autonomous case. Then, the same argument as for [25, Lemma 2.4] yields that for every $\alpha\in\mathbb{N}^{2d}$ with $|\alpha|\geq 1$ there exists a constant $C_{\boldsymbol{a},\alpha}>0$ such that

$$|\partial_{\widetilde{z}}^\alpha \widetilde{\boldsymbol{a}}(t,s,\widetilde{z})| \leq C_{\boldsymbol{a},\alpha}\ \exp(|\alpha|\,\Gamma(t,s))$$

for all $t,s\in\mathbb{R}$ and all $\widetilde{z}\in\mathbb{R}^{2d}$. In particular, $\widetilde{\boldsymbol{a}}(t,s,\cdot)$ is sublinear.

(2) Next we compare the operators $\mathrm{op}_{\mathrm{Weyl}}(\widetilde{\boldsymbol{a}}(t,s))$ and $\widetilde{\mathbf{A}}(t,s)=U(s,t)\mathbf{A}U(t,s)$. Since on the diagonal $\widetilde{\boldsymbol{a}}(t,t,\cdot)=\boldsymbol{a}$ and $U(s,s)=\mathrm{Id}$, we obtain similarly as for (2.30)

$$\begin{aligned}
&\widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}(t,s)\right)\\
&= \int_s^t U(s,\tau)\Big(\frac{\mathrm{i}}{\varepsilon}\big[H(\tau),\mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}(t,\tau)\right)\big] + \mathrm{op}_{\mathrm{Weyl}}\left(\partial_\tau\widetilde{\boldsymbol{a}}(t,\tau)\right)\Big)U(\tau,s)\,\mathrm{d}\tau\\
&= \int_s^t U(s,\tau)\Big(\mathrm{op}_{\mathrm{Weyl}}(\{h(\tau),\widetilde{\boldsymbol{a}}(t,\tau)\}) + \mathrm{op}_{\mathrm{Weyl}}\left(\partial_\tau\widetilde{\boldsymbol{a}}(t,\tau)\right)\Big)U(\tau,s)\,\mathrm{d}\tau + \rho(t,s),
\end{aligned}$$

where the last equation relies on the product rule of Weyl quantization [122, Theorem]. Here,

$$\begin{aligned}
\{h(\tau),\widetilde{\boldsymbol{a}}(t,\tau)\} &= \nabla_{\widetilde{p}}h(\tau)\cdot\nabla_{\widetilde{q}}\widetilde{\boldsymbol{a}}(t,\tau) - \nabla_{\widetilde{q}}h(\tau)\cdot\nabla_{\widetilde{p}}\widetilde{\boldsymbol{a}}(t,\tau)\\
&= \nabla_{\widetilde{z}}h(\tau)\cdot J\nabla_{\widetilde{z}}\widetilde{\boldsymbol{a}}(t,\tau)
\end{aligned}$$

denotes the Poisson bracket of $h(\tau)$ and $\widetilde{\boldsymbol{a}}(t,\tau)$. It remains to show that the integral vanishes and that the remainder $\rho(t,s)$ is of order ε^2.

(3) For the estimation of the remainder, we use that

$$\rho(t,s) = \varepsilon^2\int_s^t U(s,\tau)\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{r}(t,\tau))U(\tau,s)\,\mathrm{d}\tau,$$

where $\boldsymbol{r}(t,\tau,\cdot)$ is a smooth function depending on the derivatives of the order ≥ 3 of the function $h(\tau,\cdot)$ and of the sublinear $\widetilde{\boldsymbol{a}}(t,\tau,\cdot)$. In order to estimate

$$\left\|\rho(t,s)\varphi\right\|_{L^2} \leq \varepsilon^2\int_s^t \left\|\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{r}(t,\tau))U(\tau,s)\varphi\right\|_{L^2}\mathrm{d}\tau,$$

we investigate the above integrand.

(i) If h is subquadratic, then, due to the estimates given in (a), for all $\alpha\in\mathbb{N}_0^{2d}$ there exist $c_{1,\alpha},c_{2,\alpha}>0$ such that

$$|\partial_{\widetilde{z}}^\alpha \boldsymbol{r}(t,\tau,\widetilde{z})| \leq c_{1,\alpha}\exp(c_{2,\alpha}|t-\tau|)$$

for all $t, \tau \in \mathbb{R}$ and $\widetilde{z} \in \mathbb{R}^{2d}$, and the Calderón–Vaillancourt Theorem, see e.g. [122, Theorem 4], provides the claimed constant $C > 0$ for part (a).

(*ii*) In the magnetic case, we rewrite the remainder function

$$\boldsymbol{r}(\widetilde{q},\widetilde{p}) = \boldsymbol{r}(\cdot,\cdot,\widetilde{q},\widetilde{p}) = \boldsymbol{b}_0(\widetilde{q},\widetilde{p}) + \boldsymbol{b}(\widetilde{q},\widetilde{p})^T\widetilde{p},$$

where $\boldsymbol{b}_0 : \mathbb{R}\times\mathbb{R}\times\mathbb{R}^{2d} \to \mathbb{R}$ and $\boldsymbol{b} : \mathbb{R}\times\mathbb{R}\times\mathbb{R}^{2d} \to \mathbb{R}^d$ are bounded with all their derivatives. For the first summand, we proceed as in the subquadratic case, using Calderón–Vaillancourt. For the second summand containing an unbounded linearity in $\widetilde{p}$, we use the product rule and obtain that

$$\mathrm{op}_{\mathrm{Weyl}}\big(\boldsymbol{r}_2(\widetilde{q},\widetilde{p})\big) = -\mathrm{op}_{\mathrm{Weyl}}\big(\boldsymbol{b}(\widetilde{q},\widetilde{p})\big)\cdot \mathrm{i}\varepsilon\nabla + \mathcal{O}(\varepsilon).$$

Then, the boundedness of $\boldsymbol{b}$ provides $C_{\boldsymbol{b}} > 0$ such that

$$\big\|\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{b}(t,\tau))\varepsilon\nabla\big(U(\tau,s)\varphi\big)\big\|_{L^2} \le C_{\boldsymbol{b}}\big\|\varepsilon\nabla\big(U(\tau,s)\varphi\big)\big\|_{L^2}.$$

In the next step, we analyse $\big\|\varepsilon\nabla\big(U(\tau,s)\varphi\big)\big\|_{L^2}$.

(4) Let $t \ge s$ and set $f(t) = \mathrm{op}_{\mathrm{Weyl}}(\widetilde{z})U(t,s)\varphi$. We argue as in the proof for [35, Lemma 10.4] and observe that $f(t)$ solves the perturbed magnetic Schrödinger equation

$$\mathrm{i}\varepsilon\partial_t f(t) = \mathrm{op}_{\mathrm{Weyl}}(\widetilde{z})H(t)U(t,s)\varphi = H(t)f(t) + \delta(t)$$

with source term

$$\delta(t) = [\mathrm{op}_{\mathrm{Weyl}}(\widetilde{z}), H(t)]U(t,s)\varphi = \frac{\varepsilon}{\mathrm{i}}\begin{pmatrix}\mathrm{op}_{\mathrm{Weyl}}(\widetilde{p} - A(\widetilde{q}))\\ \mathrm{op}_{\mathrm{Weyl}}\big(\nabla\widetilde{V}(\widetilde{q}) - \nabla A(\widetilde{q})\cdot\widetilde{p}\big)\end{pmatrix}U(t,s)\varphi,$$

where we used the product rule for the second equation. In the same spirit as in step (3), we estimate

$$\big\|\delta(t)\big\|_{L^2} \le C\varepsilon\big\|\mathrm{op}_{\mathrm{Weyl}}(\widetilde{z})U(t,s)\varphi\big\|_{L^2} = C\varepsilon\big\|f(t)\big\|_{L^2},$$

where we exploited the sublinearity of A and that $\widetilde{V}$ is subquadratic. By the variation of constants formula followed by Gronwall's lemma, we obtain that

$$\big\|f(t)\big\|_{L^2} \le \mathrm{e}^{C(t-s)}\big\|f(s)\big\|_{L^2} = \mathrm{e}^{C(t-s)}\big\|\mathrm{op}_{\mathrm{Weyl}}(\widetilde{z})\varphi\big\|_{L^2}.$$

(5) In the following step we show that $\widetilde{\boldsymbol{a}}$ satisfies the transport equation

$$\partial_\tau\widetilde{\boldsymbol{a}}(t,\tau) = -\{h(\tau),\widetilde{\boldsymbol{a}}(t,\tau)\}, \tag{2.33a}$$

$$\widetilde{\boldsymbol{a}}(t,t) = \boldsymbol{a} \tag{2.33b}$$

for $\tau \in [s,t]$. Then the integrand in question indeed vanishes, and we obtain

$$\widetilde{\mathbf{A}}(t,s) = \mathrm{op}_{\mathrm{Weyl}}(\widetilde{\boldsymbol{a}}(t,s)) + \mathcal{O}(\varepsilon^2),$$

as claimed. We rewrite the transport equation (2.33) as

$$\begin{aligned}\partial_\tau\widetilde{\boldsymbol{a}}(t,\tau) &= J\nabla_{\widetilde{z}}h(\tau)\cdot\nabla_{\widetilde{z}}\widetilde{\boldsymbol{a}}(t,\tau),\\ \widetilde{\boldsymbol{a}}(t,t) &= \boldsymbol{a}.\end{aligned} \tag{2.34}$$

The following argument crucially uses that $\Phi^{t,\tau}$ is a diffeomorphism with inverse $(\Phi^{t,\tau})^{-1} = \Phi^{\tau,t}$. We observe that $\widetilde{\boldsymbol{a}}(t,\tau,\Phi^{\tau,t}(\widetilde{z})) = \boldsymbol{a}(\widetilde{z})$ for all $\widetilde{z} \in \mathbb{R}^{2d}$ and calculate

$$\begin{aligned} 0 &= \partial_\tau \boldsymbol{a}(\widetilde{z}) \\ &= \partial_\tau \widetilde{\boldsymbol{a}}(t,\tau,\Phi^{\tau,t}(\widetilde{z})) \\ &= (\partial_\tau \widetilde{\boldsymbol{a}})(t,\tau,\Phi^{\tau,t}(\widetilde{z})) - J(\nabla_{\widetilde{z}} h)(\tau,\Phi^{\tau,t}(\widetilde{z})) \cdot (\nabla_{\widetilde{z}} \widetilde{\boldsymbol{a}})(t,\tau,\Phi^{\tau,t}(\widetilde{z})), \end{aligned}$$

where, we used in the last step, the chain rule and (2.31). Since $\Phi^{\tau,t}$ is a diffeomorphism, this proves that $\widetilde{\boldsymbol{a}}(t,\tau)$ indeed solves the transport equation (2.34). □

2.7.3 Averages with respect to Gaussian wave packets

The a posteriori error representation of Lemma 2.20 involves an average with respect to the variational solution. By Egorov's theorem, Proposition 2.21, the time-evolved quantum observable can be approximated by the Weyl-quantized classical observable evolved along the classical flow. We therefore derive an asymptotic expansion of averages of Weyl-quantized operators with respect to Gaussian wave packets. For obtaining this expansion, the following phase space moments will be useful.

Lemma 2.22 (Gaussian moments)**.** *We consider a Gaussian $u \in \mathcal{M}$ of unit norm, $\|u\| = 1$, with phase space center $z = (q,p) \in \mathbb{R}^{2d}$ and width matrix $\mathcal{C} \in \mathbb{C}^{d\times d}$. We denote by*

$$\rho_\ell(\mathcal{C}) = \pi^{-d} \int_{\mathbb{R}^{2d}} \widetilde{z}^\ell \exp(-\widetilde{z}\cdot G\widetilde{z})\,\mathrm{d}\widetilde{z} \quad \text{with} \quad G = \begin{pmatrix} \mathcal{C}_\mathrm{I} + \mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\mathcal{C}_\mathrm{R} & -\mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1} \\ \mathcal{C}_\mathrm{I}^{-1}\mathcal{C}_\mathrm{R} & \mathcal{C}_\mathrm{I}^{-1} \end{pmatrix},$$

where $G \in \mathbb{R}^{2d\times 2d}$ is symmetric, positive definite and symplectic. Then, for any multi-index $\ell = (\ell_1,\dots,\ell_{2d}) \in \mathbb{N}_0^{2d}$, we have

$$\langle (\widetilde{z}-z)^\ell \rangle_u = \varepsilon^{|\ell|/2} \rho_\ell(\mathcal{C}).$$

If the length $|\ell|$ of the multi-index is odd, then we have $\langle (\widetilde{z}-z)^\ell \rangle_u = 0$.

Proof. The claimed representation becomes evident, when using the Wigner function of the Gaussian wave packet u. The Wigner function of a Gaussian wave packet centered in z satisfies

$$\mathcal{W}_u(\widetilde{z}) = (\pi\varepsilon)^{-d} \exp(-\tfrac{1}{\varepsilon}(\widetilde{z}-z)\cdot G(\widetilde{z}-z)),$$

where the matrix G is symplectic, symmetric, positive definite, see [87, Proposition 6.15]. The average of any Weyl-quantized observable can be written as the phase space integral of the symbol versus the Wigner function, see for example [87, Theorem 6.5]. In particular,

$$\begin{aligned} \langle (\widetilde{z}-z)^\ell \rangle_u &= \int_{\mathbb{R}^{2d}} (\widetilde{z}-z)^\ell \,\mathcal{W}_u(\widetilde{z})\,\mathrm{d}\widetilde{z} \\ &= (\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} (\widetilde{z}-z)^\ell \exp(-\tfrac{1}{\varepsilon}(\widetilde{z}-z)\cdot G(\widetilde{z}-z))\,\mathrm{d}\widetilde{z} \\ &= \pi^{-d}\varepsilon^{|\ell|/2} \int_{\mathbb{R}^{2d}} \widetilde{z}^\ell \exp(-\widetilde{z}\cdot G\widetilde{z})\,\mathrm{d}\widetilde{z}, \end{aligned}$$

where we have used that symplecticity implies $\det(G) = 1$. We observe, that if the length $|\ell|$ of the multi-index is odd, then the above integral vanishes, and consequently $\langle (\widetilde{z}-z)^\ell \rangle_u = 0$ as well. □

We now use these moments for expanding Gaussian averages with respect to general observables.

Proposition 2.23 (Gaussian averages)**.** *We consider a Gaussian $u \in \mathcal{M}$ of unit norm, $\|u\| = 1$, with phase space center $z = (q,p) \in \mathbb{R}^{2d}$ and complex width matrix $\mathcal{C} \in \mathbb{C}^{d\times d}$. Then, for any smooth function $\boldsymbol{a} : \mathbb{R}^{2d} \to \mathbb{R}$ with bounded sixth order derivatives,*

$$\langle \boldsymbol{a} \rangle_u = \boldsymbol{a}(z) + \varepsilon f_2(\boldsymbol{a},\mathcal{C}) + \varepsilon^2 f_4(\boldsymbol{a},\mathcal{C}) + \rho^\varepsilon(\boldsymbol{a},\mathcal{C}),$$

where

$$f_k(\boldsymbol{a},\mathcal{C}) = \sum_{|\ell|=k} \frac{1}{\ell!}\, \partial^\ell \boldsymbol{a}(z)\, \rho_\ell(\mathcal{C}), \qquad k = 2,4.$$

The second order contribution satisfies

$$f_2(\boldsymbol{a},\mathcal{C}) = \tfrac{1}{4}\mathrm{tr}(\nabla^2 \boldsymbol{a}(z)_{\mathcal{C}}\, {\mathcal{C}_{\mathrm{I}}}^{-1})$$

with

$$\nabla^2 \boldsymbol{a}(z)_{\mathcal{C}} = \begin{pmatrix} \mathrm{Id} & \mathcal{C}^* \end{pmatrix} \nabla^2 \boldsymbol{a}(z) \begin{pmatrix} \mathrm{Id} \\ \mathcal{C} \end{pmatrix} \in \mathbb{C}^{d\times d}. \tag{2.35}$$

The remainder satisfies $|\rho^\varepsilon(\boldsymbol{a},\mathcal{C})| \le C\varepsilon^3$ with a constant $C > 0$ that only depends on sixth order derivatives of $\boldsymbol{a}$ as well as on the width matrix $\mathcal{C}$.

Proof. We start by Taylor expanding the symbol around z with sixth order remainder,

$$\boldsymbol{a}(\widetilde{z}) = \sum_{|k|\le 5} \frac{1}{k!} \partial^k \boldsymbol{a}(z)(\widetilde{z}-z)^k + \boldsymbol{r}_6(\widetilde{z};z),$$

where

$$\boldsymbol{r}_6(\widetilde{z};z) = \sum_{|k|=6} r_k(\widetilde{z};z)(\widetilde{z}-z)^k, \qquad r_k(\widetilde{z};z) = \frac{6}{k!}\int_0^1 (1-\vartheta)^5 \partial^k \boldsymbol{a}(z+\vartheta(\widetilde{z}-z))\, \mathrm{d}\vartheta.$$

We have

$$\langle \boldsymbol{r}_6(\widetilde{z};z)\rangle_u = \sum_{|k|=6} \int_{\mathbb{R}^{2d}} r_k(\widetilde{z};z)\, (\widetilde{z}-z)^k\, \mathcal{W}_u(\widetilde{z})\, \mathrm{d}\widetilde{z}.$$

Therefore, using Lemma 2.22,

$$\langle \boldsymbol{a} \rangle_u = \boldsymbol{a}(z) + \varepsilon f_2(\boldsymbol{a},\mathcal{C}) + \varepsilon^2 f_4(\boldsymbol{a},\mathcal{C}) + \langle \boldsymbol{r}_6(\widetilde{z};z)\rangle_u,$$

and, with the same substitution as in the proof of Lemma 2.22, we bound

$$|\langle \boldsymbol{r}_6(\widetilde{z};z)\rangle_u| \le C(\boldsymbol{a},\mathcal{C})\,\varepsilon^3 \quad \text{with} \quad C(\boldsymbol{a},\mathcal{C}) = \sum_{|k|=6} \|r_k(\cdot;z)\|_\infty\ |\rho_k(\mathcal{C})|\,.$$

The constant $C(\boldsymbol{a},\mathcal{C}) > 0$ depends on fourth order derivatives of $\boldsymbol{a}$ and on the width matrix $\mathcal{C}$. It remains to rewrite the second order contribution as

$$\begin{aligned} f_2(\boldsymbol{a},\mathcal{C}) &= \pi^{-d} \sum_{|\ell|=2} \frac{1}{\ell!} \partial^\ell \boldsymbol{a}(z) \int_{\mathbb{R}^{2d}} (G^{-1/2}\widetilde{z})^\ell \exp(-|\widetilde{z}|^2)\, \mathrm{d}\widetilde{z} \\ &= \frac{1}{2}\, \pi^{-d} \int_{\mathbb{R}^{2d}} \widetilde{z}\cdot G^{-1/2}\nabla^2 \boldsymbol{a}(z) G^{-1/2}\widetilde{z}\ \exp(-|\widetilde{z}|^2)\, \mathrm{d}\widetilde{z} \\ &= \frac{1}{4}\, \mathrm{tr}(\nabla^2 \boldsymbol{a}(z) G^{-1}). \end{aligned}$$

Since G is symplectic and symmetric, its inverse satisfies

$$G^{-1} = JGJ^{-1} = \begin{pmatrix} \mathcal{C}_{\mathrm{I}}^{-1} & \mathcal{C}_{\mathrm{I}}^{-1}\mathcal{C}_{\mathrm{R}} \\ \mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1} & \mathcal{C}_{\mathrm{I}} + \mathcal{C}_{\mathrm{R}}\mathcal{C}_{\mathrm{I}}^{-1}\mathcal{C}_{\mathrm{R}} \end{pmatrix}.$$

We decompose the Hessian $\nabla^2 \boldsymbol{a}(z)$ in block form as

$$\nabla^2 \boldsymbol{a}(z) = \begin{pmatrix} A & B \\ B^T & D \end{pmatrix}. \tag{2.36}$$

Using the cyclicity of the trace, we calculate that

$$\begin{aligned} \mathrm{tr}(\nabla^2 \boldsymbol{a}(z) G^{-1}) &= \mathrm{tr}((A + B\mathcal{C}_{\mathrm{R}} + \mathcal{C}_{\mathrm{R}} B^T + \mathcal{C}_{\mathrm{I}} D \mathcal{C}_{\mathrm{I}} + \mathcal{C}_{\mathrm{R}} D \mathcal{C}_{\mathrm{R}}) \mathcal{C}_{\mathrm{I}}^{-1}) \\ &= \mathrm{tr}(\nabla^2 \boldsymbol{a}(z)_{\mathcal{C}}\, \mathcal{C}_{\mathrm{I}}^{-1}), \end{aligned}$$

where $\nabla^2 \boldsymbol{a}(z)_{\mathcal{C}}$ was defined in (2.35) and has the form

$$\nabla^2 \boldsymbol{a}(z)_{\mathcal{C}} = A + B\mathcal{C} + \mathcal{C}^* B^T + \mathcal{C}^* D \mathcal{C},$$

which gives the claim. □

For our analysis of the observable error, we will use Proposition 2.23 also for observables that are products of two functions. One of the factors will have a controlled semiclassical expansion, when evaluated in the position center of the variational solution.

Corollary 2.24 (Gaussian averages)**.** *In the situation of Proposition 2.23 applied to a sublinear classical observable $\boldsymbol{a} : \mathbb{R}^{2d} \to \mathbb{R}$, we additionally consider a smooth and subquadratic function $b^\varepsilon : \mathbb{R}^d \to \mathbb{R}$, $x \mapsto b^\varepsilon(x)$. Then,*

$$f_2(b^\varepsilon, \mathcal{C}) = \tfrac{1}{4}\mathrm{tr}(\nabla^2 b^\varepsilon(q) {\mathcal{C}_{\mathrm{I}}}^{-1}).$$

(a) If the function satisfies

$$b^\varepsilon(q), \nabla b^\varepsilon(q) = \mathcal{O}(\varepsilon),$$

then

$$\langle \boldsymbol{a} b^\varepsilon \rangle_u = \boldsymbol{a}(z)\,(b^\varepsilon(q) + \varepsilon f_2(b^\varepsilon, \mathcal{C})) + \mathcal{O}(\varepsilon^2).$$

(b) If the function satisfies

$$b^\varepsilon(q) = \mathcal{O}(\varepsilon^2), \quad \nabla b^\varepsilon(q), \nabla^2 b^\varepsilon(q) = \mathcal{O}(\varepsilon),$$

then

$$\begin{aligned} \langle \boldsymbol{a} b^\varepsilon \rangle_u = \boldsymbol{a}(z) \big(b^\varepsilon(q) + \varepsilon f_2(b^\varepsilon, \mathcal{C}) + \varepsilon^2 f_4(b^\varepsilon, \mathcal{C})\big) \\ + \varepsilon F_{1,1}(\boldsymbol{a}, b^\varepsilon, \mathcal{C}) + \varepsilon^2 F_{1,3}(\boldsymbol{a}, b^\varepsilon, \mathcal{C}) + \mathcal{O}(\varepsilon^3) \end{aligned}$$

with

$$F_{1,n}(\boldsymbol{a}, b^\varepsilon, \mathcal{C}) = \sum_{|\ell|=n+1} \sum_{\beta \le \ell, |\beta|=1} \frac{1}{(\ell-\beta)!}\, \partial^\beta \boldsymbol{a}(z)\; \partial^{\ell-\beta} b^\varepsilon(q)\; \rho_\ell(\mathcal{C}), \quad n = 1, 3.$$

Proof. For the trace formula, it is enough to observe that the matrices B and D in the block matrix (2.36) vanish, since b^ε only depends on x.

For proving the expansions of the averages, we crucially use the Leibniz formula for the ℓth derivative of the product, that is,

$$\partial^\ell(\boldsymbol{a}b^\varepsilon)(z) = \sum_{\beta\le\ell} \binom{\ell}{\beta}\, \partial^\beta \boldsymbol{a}(z)\, \partial^{\ell-\beta} b^\varepsilon(q)$$

for any multi-index $\ell \in \mathbb{N}_0^{2d}$.

(a) In the situation of statement (a), we only consider $|\ell| = 2$ and obtain

$$\varepsilon\partial^\ell(\boldsymbol{a}b^\varepsilon)(z) = \varepsilon\boldsymbol{a}(z)\partial^\ell b^\varepsilon(q) + \mathcal{O}(\varepsilon^2).$$

Then, Proposition 2.23 implies

$$\begin{aligned}\langle \boldsymbol{a}b^\varepsilon\rangle_u &= \boldsymbol{a}(z)b^\varepsilon(q) + \varepsilon f_2(\boldsymbol{a}b^\varepsilon, \mathcal{C}) + \mathcal{O}(\varepsilon^2)\\ &= \boldsymbol{a}(z)\left(b^\varepsilon(q) + \varepsilon f_2(b^\varepsilon, \mathcal{C})\right) + \mathcal{O}(\varepsilon^2).\end{aligned}$$

(b) In the situation of statement (b), we aim for a higher order expansion and need to consider second and fourth derivatives. In the same spirit as the proof of part (a), Proposition 2.23 implies the claimed expansion of the average $\langle \boldsymbol{a}b^\varepsilon\rangle_u$.

□

Remark 2.25. The estimates of Corollary 2.24 also apply to functions $b^\varepsilon(x)$ of the form $b^\varepsilon(x) = B^\varepsilon(x)\cdot(x-q)$, where $B^\varepsilon(x) \in \mathbb{R}^d$ is sublinear with uniform bounds in ε. A derivative $\partial^\alpha b^\varepsilon(x)$ additively decomposes into a bounded function and the function $\partial^\alpha B^\varepsilon(x)\cdot(x-q)$, which can be controlled by the arguments used in the proof of Theorem 2.13 (a).

2.7.4 Proof of Theorem 2.15

We now have everything at hand to estimate the error of observables and to conclude our final main result. In the following proof, we use Assumption 2.1 on the potentials and the representation (2.29) of the remainder potential W_u only to the extent that the arguments literally also apply to the dynamics induced by general subquadratic hamiltonians. Thus, the proof improves known observable error estimates in full generality.

Proof of Theorem 2.15. By Lemma 2.20 we only have to bound the commutator in the representation formula (2.28).

(a) We start by recalling, that in the proof of Theorem 2.13, we have estimated

$$\left\|W_{u(s)}u(s)\right\|_{L^2} = \left\|(\mathrm{Id} - P_{u(s)})H(s)u(s)\right\|_{L^2} \le C\varepsilon^{3/2}. \tag{2.37}$$

(b) We denote $\widetilde{\boldsymbol{a}}(t,s) = \boldsymbol{a}\circ\Phi^{t,s}$ and expand

$$\begin{aligned}&\frac{1}{\mathrm{i}\varepsilon}\langle \overline{W}_{u(s)}\widetilde{\mathbf{A}}(t,s) - \widetilde{\mathbf{A}}(t,s)W_{u(s)}\rangle_{u(s)}\\ &= \frac{1}{\mathrm{i}\varepsilon}\langle \overline{W}_{u(s)}\mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}(t,s)\right) - \mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}(t,s)\right)W_{u(s)}\rangle_{u(s)} + r_1(s,t).\end{aligned}$$

Using first Cauchy-Schwarz and then (2.37) together with Proposition 2.21 and norm conservation, we bound the remainder by

$$|r_1(s,t)| \leq \frac{2}{\varepsilon} \left\| W_{u(s)} u(s) \right\|_{L^2} \left\| \left(\widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}(t,s)\right) \right) u(s) \right\|_{L^2} \leq c\,\varepsilon^{5/2}.$$

(c) As in the proof of Proposition 2.21, we use the product rule of Weyl calculus and expand the commutator. For notational simplicity, we suppress the dependence on t and s. We have by symmetry of the real part with respect to the L^2 scalar product and anti-symmetry of the Poisson bracket

$$\begin{aligned} &\left\langle \overline{W}_u \,\mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}\right) - \mathrm{op}_{\mathrm{Weyl}}\left(\widetilde{\boldsymbol{a}}\right) W_u \right\rangle_u \\ &= \frac{2}{\mathrm{i}} \left\langle \mathrm{Im}\, W_u \widetilde{\boldsymbol{a}} \right\rangle_u + \frac{\varepsilon}{\mathrm{i}} \left\langle \{\mathrm{Re}\, W_u, \widetilde{\boldsymbol{a}}\} \right\rangle_u + \frac{\varepsilon^2}{4\mathrm{i}} \left\langle \nabla^2 \mathrm{Im}\, W_u J \nabla^2 \widetilde{\boldsymbol{a}} J \right\rangle_u + \mathcal{O}(\varepsilon^3), \end{aligned}$$

where the constant in $\mathcal{O}(\varepsilon^3)$ depends on phase space derivatives of the remainder potential $W_{u(s)}$ and of $\widetilde{\boldsymbol{a}}(t,s)$ of the order ≥ 3. Since $\widetilde{\boldsymbol{a}}(t,s)$ is sublinear and $W_{u(s)}$ consists of subquadratic summands and a non-subquadratic summand which can be handled by Remark 2.25, the Calderón–Vaillancourt Theorem applies for the remainder term. We will prove below that

$$\left\langle \mathrm{op}_{\mathrm{Weyl}}\left(\mathrm{Im}\, W_u \widetilde{\boldsymbol{a}}\right) \right\rangle_u = \mathcal{O}(\varepsilon^3), \tag{2.38a}$$

$$\left\langle \mathrm{op}_{\mathrm{Weyl}}\left(\{\mathrm{Re}\, W_u, \widetilde{\boldsymbol{a}}\}\right) \right\rangle_u = \mathcal{O}(\varepsilon^2), \tag{2.38b}$$

$$\left\langle \mathrm{op}_{\mathrm{Weyl}}\left(\nabla^2 \mathrm{Im}\, W_u J \nabla^2 \widetilde{\boldsymbol{a}} J\right) \right\rangle_u = \mathcal{O}(\varepsilon), \tag{2.38c}$$

which allows us to conclude that

$$\frac{1}{\mathrm{i}\varepsilon} \left\langle \overline{W}_u \widetilde{\mathbf{A}} - \widetilde{\mathbf{A}} W_u \right\rangle_u = \mathcal{O}(\varepsilon^2).$$

In order to do so, we first aim at the application of Corollary 2.24 statement (a) for $b^\varepsilon = \partial_j \mathrm{Re}\, W_u$ and statement (b) for $b^\varepsilon = \mathrm{Im}\, W_u$; see also Remark 2.25 for the non-subquadratic terms in W_u.

(d) From now on, we notationally focus on the magnetic Schrödinger case, but the analysis works the same for the general case. We denote the phase space center of the variational Gaussian u by $z = (q,p)$. The width matrix of u is $\mathcal{C}$ and has imaginary part $\mathcal{C}_\mathrm{I}$. We recall that the cubic remainder $R(X_u)$ in (2.29) vanishes together with its first and second derivatives when evaluated in q.

We first apply the analysis to the Poisson bracket that involves the real part of the remainder potential. For any $j = 1, \ldots, d$, we use (2.29) and Proposition 2.23 and obtain $\partial_j \mathrm{Re}\, W_u(q) = \mathcal{O}(\varepsilon)$. Furthermore, by [87, Lemma 3.15] we have

$$\begin{aligned} \nabla \partial_j \mathrm{Re}\, W_u(q) &= \nabla \partial_j \mathrm{Re}\, X_u(q) - \langle \nabla \partial_j \mathrm{Re}\, X_u \rangle_u = \mathcal{O}(\varepsilon), \\ \nabla^2 \partial_j \mathrm{Re}\, W_u(q) &= \nabla^2 \partial_j \mathrm{Re}\, R(X_u)(q) = \nabla^2 \partial_j \mathrm{Re}\, X_u(q). \end{aligned}$$

Hence, the function $b^\varepsilon = \partial_j \mathrm{Re}\, W_u$ fulfills the assumptions of statement (a) in Corollary 2.24, and together with Proposition 2.23, we obtain

$$\langle \partial_j \mathrm{Re}\, W_u \partial_{p_j} \widetilde{\boldsymbol{a}} \rangle_u = \mathcal{O}(\varepsilon^2).$$

After summation over j, we have proven (2.38b).

(e) Similarly, the first and second derivatives of $\mathrm{Im}\, W_u$ satisfy

$$\nabla \mathrm{Im}\, W_u(q), \;\; \nabla^2 \mathrm{Im}\, W_u(q) = \mathcal{O}(\varepsilon). \tag{2.39}$$

Moreover, Proposition 2.23 implies for the point evaluation of the imaginary part of the remainder potential that

$$\begin{aligned}\operatorname{Im} W_u(q) &= \frac{\varepsilon}{4}\operatorname{tr}\big(\big(\langle\nabla^2\operatorname{Im} X_u\rangle_u - \nabla^2\operatorname{Im} X_u(q)\big)\,{\mathcal{C}_{\mathrm{I}}}^{-1}\big) + \mathcal{O}(\varepsilon^2)\\ &= \mathcal{O}(\varepsilon^2).\end{aligned} \tag{2.40}$$

At this point, a simple application of Proposition 2.23 and (2.39) yields (2.38c).

(f) The expansions in (2.39) and (2.40) show that $b^\varepsilon = \operatorname{Im} W_u$ satisfies the assumptions of statement (b) in Corollary 2.24. In order to prove (2.38a), we analyse the expansion obtained from Corollary 2.24 in two steps, aiming at

$$\operatorname{Im} W_u(q) + \varepsilon f_2(\operatorname{Im} W_u, \mathcal{C}) + \varepsilon^2 f_4(\operatorname{Im} W_u, \mathcal{C}) = \mathcal{O}(\varepsilon^3), \tag{2.41a}$$

$$\varepsilon F_{1,1}(\widetilde{\boldsymbol{a}}, \operatorname{Im} W_u, \mathcal{C}) + \varepsilon^2 F_{1,3}(\widetilde{\boldsymbol{a}}, \operatorname{Im} W_u, \mathcal{C}) = \mathcal{O}(\varepsilon^3). \tag{2.41b}$$

(g) We start with proving the first estimate (2.41a). For this, we need a slightly more accurate assessment of $\operatorname{Im} W_u(q)$ than developed previously. Using (2.29), Proposition 2.23, and (2.39), we have

$$\begin{aligned}\operatorname{Im} W_u(q) &= -\varepsilon f_2(\operatorname{Im} X_u, \mathcal{C}) - \varepsilon^2 f_4(\operatorname{Im} X_u, \mathcal{C}) + \varepsilon f_2(\langle\operatorname{Im} X_u\rangle_u, \mathcal{C}) + \mathcal{O}(\varepsilon^3)\\ &= -\varepsilon^2 f_4(\operatorname{Im} X_u, \mathcal{C}) + \varepsilon^2 f_2(f_2(\operatorname{Im} X_u, \mathcal{C}), \mathcal{C}) + \mathcal{O}(\varepsilon^3).\end{aligned}$$

Similarly, we obtain for the second term in (2.41a) that

$$\varepsilon f_2(\operatorname{Im} W_u, \mathcal{C}) = -\varepsilon^2 f_2(f_2(\operatorname{Im} X_u, \mathcal{C}), \mathcal{C}) + \mathcal{O}(\varepsilon^3).$$

Therefore, $\operatorname{Im} W_u(q)$ cancels both the contributions from the second and the fourth derivatives, and we have proven (2.41a).

(h) We next target the terms on the left hand side of equation (2.41b), that is,

$$\varepsilon F_{1,1}(\widetilde{\boldsymbol{a}}, \operatorname{Im} W_u, \mathcal{C}) = -\varepsilon^2 \sum_{|k|=2} F_{1,1}(\widetilde{\boldsymbol{a}}, \partial^k \operatorname{Im} X_u, \mathcal{C})\ \rho_k(\mathcal{C}) + \mathcal{O}(\varepsilon^3)$$

and

$$F_{1,3}(\widetilde{\boldsymbol{a}}, \operatorname{Im} W_u, \mathcal{C}) = F_{1,3}(\widetilde{\boldsymbol{a}}, \operatorname{Im} X_u, \mathcal{C}).$$

In Lemma 2.27, we provide the combinatorial argument that shows (2.41b) as a consequence of Isserlis' theorem on the higher moments of multivariate normal distributions. Hence, we have proven $\langle \operatorname{Im} W_u \widetilde{\boldsymbol{a}}\rangle_u = \mathcal{O}(\varepsilon^3)$, that is, (2.38a). □

Remark 2.26. The crucial estimates of the previous proof, namely (2.38a) and (2.38b) are one order worse for the semiclassical Gaussian approximation, since it lacks the compensating averaging factors of the remainder potential. Therefore, for the semiclassical Gaussians only $\mathcal{O}(\varepsilon)$ observable accuracy can be expected.

2.8 Appendix: Gaussian moments

By an application of Isserlis' theorem, the fourth order Gaussian moments can be written as sums of products of second order moments. That is, for a $2d$-dimensional Gaussian random vector

$$(X_1, \dots, X_{2d}) \sim \mathcal{N}(0, G)$$

with mean zero $0 \in \mathbb{R}^{2d}$ and covariance matrix $G \in \mathbb{R}^{2d \times 2d}$, the fourth order moments satisfy

$$\begin{aligned}
&\mathbb{E}(X_i^4) = 3g_{ii}^2, \\
&\mathbb{E}(X_i^3 X_j) = 3g_{ii}g_{ij}, \\
&\mathbb{E}(X_i^2 X_j^2) = g_{ii}g_{jj} + 2g_{ij}^2 \\
&\mathbb{E}(X_i^2 X_j X_k) = g_{ii}g_{jk} + 2g_{ij}g_{ik} \\
&\mathbb{E}(X_i X_j X_k X_\ell) = g_{ij}g_{k\ell} + g_{ik}g_{j\ell} + g_{i\ell}g_{jk}
\end{aligned}$$

with $i, j, k, \ell \in \{1, \dots, 2d\}$. We crucially use this for proving that the fourth order summations that appeared in the proof of Theorem 2.15 can be expressed in terms of second order summations.

Lemma 2.27 (Resummation)**.** *For any family $(a_{\beta,m})_{\beta,m}$ of real numbers, indexed by $m \in \mathbb{N}_0^{2d}$ and $\beta \leq m$ with $|\beta| = 1$, we have*

$$\sum_{|m|=4} \sum_{\beta \leq m, |\beta|=1} \frac{1}{(m-\beta)!}\, a_{\beta,m}\, \rho_m(\mathcal{C}) = \sum_{|k|=2} \sum_{|\ell|=2} \sum_{\beta \leq \ell, |\beta|=1} \frac{1}{k!}\, a_{\beta,k+\ell}\, \rho_k(\mathcal{C})\rho_\ell(\mathcal{C}).$$

Proof. We write a multi-index $m \in \mathbb{N}_0^{2d}$ of order $|m| = 4$ as

$$m = \langle j_1 \rangle + \langle j_2 \rangle + \langle j_3 \rangle + \langle j_4 \rangle$$

with coordinates $j_1, \dots, j_4 \in \{1, \dots, 2d\}$, where the bracket $\langle j \rangle = e_j$ denotes the jth canonical basis vector of $\mathbb{R}^{2d}$. We distinguish five different cases for the order four multi-index m.

(a) m has one non-zero component, that is, $m = 4\langle j \rangle$ with $j = 1, \dots, 2d$. Then,

$$\begin{aligned}
\frac{1}{(m-\beta)!}\, a_{\beta,m}\, \rho_m(\mathcal{C}) &= \frac{1}{3!}\, a_{\langle j \rangle, 4\langle j \rangle}\, 3\rho_{2\langle j \rangle}(\mathcal{C})^2 \\
&= \frac{1}{k!}\, a_{\beta,k+\ell}\, \rho_k(\mathcal{C})\rho_\ell(\mathcal{C})
\end{aligned}$$

with $k = 2\langle j \rangle = \ell$ and $\beta = \langle j \rangle$.

(b) m has two different non-zero components, that is, $m = 3\langle j_1 \rangle + \langle j_2 \rangle$ with $j_1 \neq j_2$. In this case, m dominates two multi-indices β of order one, and generates the terms

$$\begin{aligned}
&\left(\frac{1}{2!}\, a_{\langle j_1 \rangle, m} + \frac{1}{3!}\, a_{\langle j_2 \rangle, m} \right) 3\rho_{2\langle j_1 \rangle}(\mathcal{C})\rho_{\langle j_1 \rangle + \langle j_2 \rangle}(\mathcal{C}) \\
&= \frac{1}{2!} \left(a_{\langle j_1 \rangle, m} + a_{\langle j_2 \rangle, m} \right) \rho_{2\langle j_1 \rangle}(\mathcal{C})\rho_{\langle j_1 \rangle + \langle j_2 \rangle}(\mathcal{C}) \\
&+ \frac{1}{1!}\, a_{\langle j_1 \rangle, m}\, \rho_{\langle j_1 \rangle + \langle j_2 \rangle}(\mathcal{C})\rho_{2\langle j_1 \rangle}(\mathcal{C}).
\end{aligned}$$

This amounts to the two (k, ℓ) pairs

$$\begin{aligned}
&k = 2\langle j_1 \rangle,\ \ell = \langle j_1 \rangle + \langle j_2 \rangle,\ \beta \in \{\langle j_1 \rangle, \langle j_2 \rangle\}, \\
&k = \langle j_1 \rangle + \langle j_2 \rangle,\ \ell = 2\langle j_1 \rangle,\ \beta = \langle j_1 \rangle.
\end{aligned}$$

(c) m has two identical non-zero components, that is, $m = 2\langle j_1\rangle + 2\langle j_2\rangle$ with $j_1 \neq j_2$. In this case, m again dominates two multi-indices β of order one, and we have to consider

$$\begin{aligned}
&\frac{1}{2!}\left(a_{\langle j_1\rangle,m} + a_{\langle j_2\rangle,m}\right)\left(\rho_{2\langle j_1\rangle}(\mathcal{C})\rho_{2\langle j_2\rangle}(\mathcal{C}) + 2\rho_{\langle j_1\rangle+\langle j_2\rangle}(\mathcal{C})^2\right)\\
&= \frac{1}{2!}a_{\langle j_2\rangle,m}\ \rho_{2\langle j_1\rangle}(\mathcal{C})\rho_{2\langle j_2\rangle}(\mathcal{C}) + \frac{1}{2!}a_{\langle j_1\rangle,m}\ \rho_{2\langle j_2\rangle}(\mathcal{C})\rho_{2\langle j_1\rangle}(\mathcal{C})\\
&+ \frac{1}{1!}\left(a_{\langle j_1\rangle,m} + a_{\langle j_2\rangle,m}\right)\rho_{\langle j_1\rangle+\langle j_2\rangle}(\mathcal{C})^2.
\end{aligned}$$

This amounts to the three pairs

$$\begin{aligned}
&k = 2\langle j_1\rangle,\ \ell = 2\langle j_2\rangle,\ \beta = \langle j_2\rangle\\
&k = 2\langle j_2\rangle,\ \ell = 2\langle j_1\rangle,\ \beta = \langle j_1\rangle\\
&k = \langle j_1\rangle + \langle j_2\rangle = \ell,\ \beta \in \{\langle j_1\rangle, \langle j_2\rangle\},
\end{aligned}$$

that satisfy $k + \ell = m$.

(d) m has three non-zero components, that is, $m = 2\langle j_1\rangle + \langle j_2\rangle + \langle j_3\rangle$ with pairwise distinct j_1, j_2, j_3. In this case, m dominates three multi-indices β of order one. The contributions are

$$\begin{aligned}
&\left(a_{\langle j_1\rangle,m} + \frac{1}{2!}\,a_{\langle j_2\rangle,m} + \frac{1}{2!}\,a_{\langle j_3\rangle,m}\right)\\
&\times\left(\rho_{2\langle j_1\rangle}(\mathcal{C})\rho_{\langle j_2\rangle+\langle j_3\rangle}(\mathcal{C}) + 2\rho_{\langle j_1\rangle+\langle j_2\rangle}(\mathcal{C})\rho_{\langle j_1\rangle+\langle j_3\rangle}(\mathcal{C})\right)\\
&= \frac{1}{2!}\left(a_{\langle j_2\rangle,m} + a_{\langle j_3\rangle,m}\right)\rho_{2\langle j_1\rangle}(\mathcal{C})\rho_{\langle j_2\rangle+\langle j_3\rangle}(\mathcal{C})\\
&+ \frac{1}{1!}\,a_{\langle j_1\rangle,m}\,\rho_{\langle j_2\rangle+\langle j_3\rangle}(\mathcal{C})\rho_{2\langle j_1\rangle}(\mathcal{C})\\
&+ \left(a_{\langle j_1\rangle,m} + a_{\langle j_3\rangle,m}\right)\rho_{\langle j_1\rangle+\langle j_2\rangle}(\mathcal{C})\rho_{\langle j_1\rangle+\langle j_3\rangle}(\mathcal{C})\\
&+ \left(a_{\langle j_1\rangle,m} + a_{\langle j_2\rangle,m}\right)\rho_{\langle j_1\rangle+\langle j_3\rangle}(\mathcal{C})\rho_{\langle j_1\rangle+\langle j_2\rangle}(\mathcal{C}).
\end{aligned}$$

This amounts to the four pairs

$$\begin{aligned}
&k = 2\langle j_1\rangle,\ \ell = \langle j_2\rangle + \langle j_3\rangle,\ \beta \in \{\langle j_2\rangle, \langle j_3\rangle\},\\
&k = \langle j_2\rangle + \langle j_3\rangle,\ \ell = 2\langle j_1\rangle,\ \beta = \langle j_1\rangle,\\
&k = \langle j_1\rangle + \langle j_2\rangle,\ \ell = \langle j_1\rangle + \langle j_3\rangle,\ \beta \in \{\langle j_1\rangle, \langle j_3\rangle\},\\
&k = \langle j_1\rangle + \langle j_3\rangle,\ \ell = \langle j_1\rangle + \langle j_2\rangle,\ \beta \in \{\langle j_1\rangle, \langle j_2\rangle\},
\end{aligned}$$

which satisfy $k + \ell = m$.

(e) m has four non-zero components, that is, $m = \langle j_1\rangle + \cdots + \langle j_4\rangle$ with distinct $j_1, \ldots, j_4$. In this case, m dominates four multi-indices β of order one, and we have to consider

$$\begin{aligned}
&\left(a_{\langle j_1\rangle,m} + \cdots + a_{\langle j_4\rangle,m}\right)\left(\rho_{\langle j_1\rangle+\langle j_2\rangle}(\mathcal{C})\rho_{\langle j_3\rangle+\langle j_4\rangle}(\mathcal{C}) +\right.\\
&\left.+\rho_{\langle j_1\rangle+\langle j_3\rangle}(\mathcal{C})\rho_{\langle j_2\rangle+\langle j_3\rangle}(\mathcal{C}) + \rho_{\langle j_1\rangle+\langle j_4\rangle}(\mathcal{C})\rho_{\langle j_2\rangle+\langle j_3\rangle}(\mathcal{C})\right).
\end{aligned}$$

This product results in twelve summands, that have an obvious regrouping according to the six (k,ℓ) pairs

$$\begin{aligned}
&k = \langle j_1\rangle + \langle j_2\rangle,\ \ell = \langle j_3\rangle + \langle j_4\rangle,\ \beta \in \{\langle j_3\rangle, \langle j_4\rangle\},\\
&k = \langle j_1\rangle + \langle j_3\rangle,\ \ell = \langle j_2\rangle + \langle j_4\rangle,\ \beta \in \{\langle j_2\rangle, \langle j_4\rangle\},\\
&k = \langle j_1\rangle + \langle j_4\rangle,\ \ell = \langle j_2\rangle + \langle j_3\rangle,\ \beta \in \{\langle j_2\rangle, \langle j_3\rangle\},\\
&k = \langle j_2\rangle + \langle j_3\rangle,\ \ell = \langle j_1\rangle + \langle j_4\rangle,\ \beta \in \{\langle j_1\rangle, \langle j_4\rangle\},\\
&k = \langle j_2\rangle + \langle j_4\rangle,\ \ell = \langle j_1\rangle + \langle j_3\rangle,\ \beta \in \{\langle j_1\rangle, \langle j_3\rangle\},\\
&k = \langle j_3\rangle + \langle j_4\rangle,\ \ell = \langle j_1\rangle + \langle j_2\rangle,\ \beta \in \{\langle j_1\rangle, \langle j_2\rangle\}.
\end{aligned}$$

We note, that all k have their factorials equal to one, and that $k+\ell = m$.

In the previous five cases (a)–(e), that follow the sparsity pattern of order four multi-indices, we obtain the appropriate format of the resulting summands, that is,

$$\frac{1}{k!}\sum_{\beta\le\ell,|\beta|=1} a_{\beta,k+\ell}\,\rho_k(\mathcal{C})\,\rho_\ell(\mathcal{C})$$

with $k,\ell\in\mathbb{N}_0^{2d}$ such that $|k| = |\ell| = 2$ and $k+\ell = m$. For concluding the proof, we have to verify that any possible (k,ℓ) pairing of order two multi-indices has appeared in one of the five cases (a)–(e). Let $i_1,\dots,i_4\in\{1,\dots,2d\}$ be such that

$$k = \langle i_1\rangle + \langle i_2\rangle,\quad \ell = \langle i_3\rangle + \langle i_4\rangle.$$

The combinatorics of this situation falls into the following five cases:

(α) All four coordinates agree, that is, $i_1 = \cdots = i_4 =: j$. Then, $k+\ell = 4\langle j\rangle$, and we recognize the previous case (a).

(β) Three of the four coordinates coincide with each other, that is, $i_1 = i_2 = i_3 =: j_1$ and $i_4 =: j_2$ is distinct from the other three ones, or the analogous three possible placements of an outlier. Then, $k+\ell = 3\langle j_1\rangle + \langle j_2\rangle$, which is case (b).

(γ) The four coordinates form two different pairs, that is, $i_1 = i_2 =: j_1$ and $i_3 = i_4 =: j_2$ or the other two possible pairings. Then, $k+\ell = 2\langle j_1\rangle + 2\langle j_2\rangle$, and we are in case (c).

(δ) Two of the four coordinates agree, while the other two are different. That is, $i_1 = i_2 =: j_1$ and $i_3\neq i_4$ and different to j_1, or the other two possible pairings. Then, $k+\ell = 2\langle j_1\rangle + \langle i_3\rangle + \langle i_4\rangle$, which is case (d).

(ε) All four coordinates are distinct as in case (e).

Hence, the combinatorics of the order four multi-indices and the one of pairs of order two multi-indices are the same, and we have indeed proven that the two different summation formats yield the same result as claimed. □

CHAPTER 3

Time-dependent electromagnetic scattering from dispersive materials

The content of this chapter was published in [113]. The authors are Jörg Nick, Selina Burkhard and Christian Lubich.

This chapter studies time-dependent electromagnetic scattering from obstacles that are described by dispersive material laws. We consider the numerical treatment of a scattering problem in which a dispersive material law, for a causal and passive homogeneous material, determines the wave-material interaction in the scatterer. The resulting problem is nonlocal in time inside the scatterer and is posed on an unbounded domain. Wellposedness of the scattering problem is shown using a formulation that is fully given on the surface of the scatterer via a time-dependent boundary integral equation. Discretizing this equation by convolution quadrature in time and boundary elements in space yields a provably stable and convergent method that is fully parallel in time and space. Under regularity assumptions on the exact solution we derive error bounds with explicit convergence rates in time and space. Numerical experiments illustrate the theoretical results and show the effectiveness of the method.

3.1 Introduction and setting

Since the pioneering work of [128], dispersive materials and their interaction with electromagnetic waves have attracted much scientific interest. Metamaterials, whose interaction with electromagnetic waves is often described by dispersive material laws, promises to advance many applications in the context of optical devices and imaging. A collection of applications is found in [93, Section 5].

A survey of the mathematical literature is given by [93] and a coherent presentation of basic mathematical results is given by [37]. Following that paper, we require the causality principle and homogeneity for the dispersive material law, and we consider the fundamental class of (strongly) passive materials. Studying the time domain setting of dispersive has recently been further motivated by [36], which presents a numerical study that indicates that the limiting amplitude principle does not generally hold for dispersive material laws.

In the approach to time-dependent scattering taken here, the scattering problem posed in the exterior domain and the dispersive bounded scattering object is reduced to a time-dependent boundary integral equation for the tangential traces of the electric and magnetic fields. From the tangential traces, the electromagnetic fields inside and outside the scatterer are then obtained via representation formulas. We show well-posedness of the boundary integral equation and the scattering problem for causal and passive homogeneous dispersive materials. We use convolution quadrature and boundary elements for the numerical discretization and provide a fully discrete error analysis. Numerical experiments illustrate the theoretical results and show the effectiveness of the method.

The numerical simulation of wave propagation problems on exterior domains by discretizing time-dependent boundary integral equations with convolution quadrature in time and boundary elements in space originates from [95]. This approach has been taken up in the numerical literature both in the acoustic case, e.g. [12, 13, 18, 19, 86, 123], and in the electromagnetic case, e.g. [9, 38, 40, 84, 112]. In [42], a convolution quadrature discretization has been applied to dispersive electromagnetic material laws in combination with finite volume techniques.

Further related literature is, e.g., [118], which considers the acoustic wave equation and a reformulation as retarded boundary integral equation. The discretization is provided by a Galerkin semi-discretization in space and convolution quadrature in time. In contrast to us, this paper uses evolution equation techniques for the fully discrete system. In [44], a formulation of an acoustic wave transmission problem with mixed boundary conditions as a retarded potential integral equation is derived and wellposedness is shown. [38] solve dielectric scattering with a homogeneous penetrable obstacle, by using boundary integral methods and convolution quadrature.

For a recent overview on convolution quadrature with applications to scattering problems, we refer to [14].

3.1.1 Dispersive Maxwell's equations on a single domain Ω

Let $\Omega \subset \mathbb{R}^3$ be an interior or exterior domain. We are interested in time-dependent (possibly dispersive) electromagnetic waves, which are modeled by *Maxwell's equations* (here assumed with vanishing current

and charge)

$$\begin{aligned} \partial_t \boldsymbol{D} - \mathbf{curl}\, \boldsymbol{H} &= 0 \\ \partial_t \boldsymbol{B} + \mathbf{curl}\, \boldsymbol{E} &= 0 \end{aligned} \quad \text{in } \Omega. \tag{3.1}$$

These equations are complemented by the material laws

$$\boldsymbol{D} = \varepsilon_0 \boldsymbol{E} + \boldsymbol{P}(\boldsymbol{E}), \quad \boldsymbol{B} = \mu_0 \boldsymbol{H} + \boldsymbol{M}(\boldsymbol{H}), \tag{3.2}$$

with the constant permittivity ε_0 and permeability μ_0 of vacuum and with the polarization field $\boldsymbol{P}$ and the magnetization field $\boldsymbol{M}$. For homogeneous materials, as will be considered here, these fields are of the form of a temporal convolution

$$\boldsymbol{P}(\boldsymbol{E})(t) = \varepsilon_0 \int_0^t \chi_e(\theta) \boldsymbol{E}(t-\theta)\, \mathrm{d}\theta, \tag{3.3}$$

$$\boldsymbol{M}(\boldsymbol{H})(t) = \mu_0 \int_0^t \chi_m(\theta) \boldsymbol{H}(t-t')\, \mathrm{d}\theta, \tag{3.4}$$

with the scalar susceptibility kernels χ_e and χ_m.

3.1.2 Examples of retarded material laws

We present various material laws, which can be found in [33, 37]. The reaction of material, different from vacuum, is non-instantaneous when exposed to stress. It depends on the past, it has a memory.

A common example used in the literature is the Debye model, for which the susceptibility kernel is given by

$$\chi_e(t) = \beta \mathrm{e}^{-\lambda t}, \quad \text{for} \quad \lambda, \beta > 0, \tag{3.5a}$$

with relaxation parameter $1/\lambda$. Here the distraction of the material depends stronger on the more recent past, this is captured by the exponential damping. Kernels in physical applications often consist of sums of the type given above or, more generally, are completely monotonic functions (cf. [133])

$$\chi_e(t) = \int_0^\infty \mathrm{e}^{-\lambda t} \beta(\,\mathrm{d}\lambda) \qquad \text{with a positive measure } \beta.$$

Another class of material laws simultaneously damps the system and introduces a temporal delay, by some fixed $t_* > 0$. The analysis of such systems has received significant attention, for example in [108] and, for scattering problems, in [117]. In our setting, such models are described by the convolution with the shifted Heaviside function

$$\chi_e(t) = \alpha_1 + \alpha_2 \Theta(t - t_*) = \begin{cases} \alpha_1 + \alpha_2, & t \geq t_* \\ \alpha_1, & t < t_*. \end{cases} \tag{3.5b}$$

We always assume that the parameters satisfy $\alpha_1 \geq \alpha_2 > 0$. In [108], the respective material law in the acoustic setting has been shown to be exponentially stable for $\alpha_1 > \alpha_2 > 0$. The authors further construct, for the converse case of $\alpha_2 > \alpha_1$, arbitrary small shifts t_* that destabilize the system. In the next sections we will show that the corresponding electromagnetic scattering problem is well-posed and stable under the stated constraints.

Popular models for the propagation of light and its interaction with matter are the Drude and Lorentz models in nanophotonics; see [33, 37]. The Drude model can be used to model metal under the influence

of an external electric field. Then, the conduction electrons behave as charged free particles, they form an ideal classical gas. With the collision frequency γ_D and the plasma frequency ω_D, the temporal susceptibility kernel is given by

$$\chi(t) = \frac{\omega_D^2}{\gamma_D}\left(1 - \mathrm{e}^{-\gamma_D t}\right). \tag{3.5c}$$

The Drude model has to be modified for metals in the visible regime, where interband transitions of the electrons occur due to higher photon energies. In this case Lorentz oscillators provide a simple model: with

$$\chi(t) = \frac{\beta_L}{\lambda_L}\mathrm{e}^{-\frac{\alpha_L}{2}t}\sin(\lambda_L t), \qquad \lambda_L = \sqrt{\omega_L^2 - \frac{\alpha_L}{4}}, \tag{3.5d}$$

where ω_L is the resonance frequency, $0 < \alpha_L < 4\omega_L^2$ is the damping coefficient and $\beta_L > 0$ gives the strength.

More involved models contain fractional derivatives, such as the Havriliak-Negami model, which models dielectric relaxation in complex systems, cf. [132] and [53]: with positive coefficients β and γ and the exponent $0 < \eta < 2$,

$$\varepsilon_0\big((1+\gamma)\partial_t + \beta\partial_t^{1+\eta}\big)\boldsymbol{E} - \mathbf{curl}\left(1 + \beta\partial_t^{\eta}\right)\boldsymbol{H} = 0. \tag{3.5e}$$

This can be reformulated as (3.2) with (3.3), where $\chi_e(t)$ is the convolution kernel given by its Laplace transform $\widehat{\chi}_e(s) = \gamma/(1+\beta s^\eta)$.

3.1.3 The time-dependent scattering problem

We decompose the complete space $\mathbb{R}^3$ into the exterior domain Ω^+, the interior (bounded) domain Ω^- and the interface $\Gamma = \partial\Omega^+ = \partial\Omega^-$, which yields the disjoint union $\mathbb{R}^3 = \Omega^- \cup \Gamma \cup \Omega^+$. Inside the scatterer, i.e. in the bounded domain Ω^-, we enforce a retarded material law and couple it with Maxwell's equations with physical parameters corresponding to a vacuum in the exterior domain Ω^+. We then arrive at the following equations in their respective domains:

In the interior domain Ω^-:

$$\begin{aligned} \varepsilon_0\partial_t\boldsymbol{E}^- &+ \boldsymbol{P}(\partial_t\boldsymbol{E}^-) - \mathbf{curl}\,\boldsymbol{H}^- = 0,\\ \mu_0\partial_t\,\boldsymbol{H}^- &+ \boldsymbol{M}(\partial_t\boldsymbol{H}^-) + \mathbf{curl}\,\boldsymbol{E}^- = 0. \end{aligned}$$

In the exterior domain Ω^+:

$$\begin{aligned} \varepsilon_0\partial_t\boldsymbol{E}^+ - \mathbf{curl}\,\boldsymbol{H}^+ &= 0,\\ \mu_0\partial_t\boldsymbol{H}^+ + \mathbf{curl}\,\boldsymbol{E}^+ &= 0. \end{aligned}$$

Initially, we assume the system to be at rest with vanishing electromagnetic fields in the interior and the exterior. The system is excited by an exterior incoming electromagnetic wave $(\boldsymbol{E}_{\mathrm{inc}}, \boldsymbol{H}_{\mathrm{inc}})$, a solution of the exterior Maxwell's equations with support initially away from the surface Γ of the scatterer. The unknown exterior fields $(\boldsymbol{E}^+, \boldsymbol{H}^+)$ are referred to as the *scattered fields*. They uniquely identify, together with the incoming wave, the total electromagnetic fields via $\boldsymbol{E}^{\mathrm{tot}} = \boldsymbol{E}^+ + \boldsymbol{E}_{\mathrm{inc}}$ and $\boldsymbol{H}^{\mathrm{tot}} = \boldsymbol{H}^+ + \boldsymbol{H}_{\mathrm{inc}}$. Inside the scatterer there is only the initially vanishing scattered wave $(\boldsymbol{E}^-, \boldsymbol{H}^-)$, making such a distinction unnecessary.

Along the interface of the scatterer $\Gamma = \partial\Omega^{\pm}$, we enforce continuity of the tangential components of the total electric and magnetic fields, which reads

$$\begin{aligned} \gamma_T\boldsymbol{E}^- &= \gamma_T\boldsymbol{E}^+ + \gamma_T\boldsymbol{E}^+_{\mathrm{inc}},\\ \gamma_T\boldsymbol{H}^- &= \gamma_T\boldsymbol{H}^+ + \gamma_T\boldsymbol{H}^+_{\mathrm{inc}} \end{aligned} \qquad \text{on } \Gamma. \tag{3.6}$$

The numerical treatment of this scattering problems needs to overcome the following main challenges of the problem above:

- The material laws (3.3)–(3.4) are nonlocal in time and therefore require, for general susceptibilities (χ_e, χ_m), the whole history of the solution at any time t, which leads to a memory tail with standard time-stepping discretizations.
- The exterior domain Ω^+ is unbounded.

The natural formulation of this scattering problem considers vacuum in the unbounded exterior domain. However, the case of retarded material laws in the exterior domain, as is encountered e.g. when the scattering is caused by a small inclusion in a dispersive material, does not introduce any additional difficulty. We therefore impose, for the rest of the paper, different dispersive material laws on Ω^- and Ω^+ respectively, which is a general setting that includes the natural case of a dispersive scatterer in a dielectric background medium.

3.1.4 Outline and contributions of the paper

The present problem formulation is partly inspired by [38], which gives the first numerical analysis for time-dependent electromagnetic scattering from dielectric penetrable obstacles. In this paper, we go beyond the existing literature by a thorough numerical analysis for scattering from dispersive materials, which are described by non-local convolutional material laws in the time domain and frequency-dependent permittivities and permeabilities in the Laplace domain. The mathematical theory describing such materials has been extensively developed in the last years, see for example [37] for an excellent overview.

We transfer the techniques developed in [84] and [112], which in turn originate in the acoustic analogues of [18] and [19], respectively. On the analytical side, we show that the assumptions made on the mathematical models for dispersive materials lead to well-posed boundary integral equations. On the numerical side, employing a temporal discretization based on the convolution quadrature method combined with a boundary element space discretization, we provide the first provably stable and convergent numerical method for time-dependent electromagnetic scattering from dispersive materials based on time-dependent boundary integral equations. In the following, we give an outline and discuss the contributions of each section.

In Section 4.2, we recall the foundation of dispersive Maxwell's equations and describe the framework of passive material laws used in the subsequent sections. Lemma 3.1 shows that all examples from the introduction are included in the setting.

Section 3.3 formulates and analyses a basic dispersive time-harmonic transmission problem, for which a central bound for the electromagnetic fields is shown in Lemma 3.3. As a consequence, bounds for the potential and boundary operators corresponding to the time-harmonic dispersive Maxwell's equations are deduced. Moreover, the fundamental Calderón operator is constructed for the dispersive Maxwell's equations, which is differently scaled than its dielectric counterpart in the previous work by [84]. Assuming passivity of the material law, we obtain the crucial time-harmonic coercivity result of Lemma 3.6.

In Section 3.4, we apply the previously established operators to derive a well-posed and stable time-harmonic boundary integral equation and prove the equivalence to the time-harmonic scattering problem of interest in Proposition 3.10. Moreover, s-specific bounds are shown which estimate the solution of

the scattering problem in terms of the incoming wave. Assuming a stronger passivity assumption on the material law, we obtain simplified bounds of all operators, which can be transported into the time-domain.

Section 3.5 carries the time-harmonic analysis over to the time-domain. The time-dependent boundary integral equation is formulated in (3.35) and its central properties are collectively shown in Theorem 3.13. In particular, we show the wellposedness of the boundary integral equation, the equivalence to the time-dependent scattering problem and give estimates on the solution in terms of the incoming waves. All of these results are the direct consequence of their time-harmonic counterparts.

In Section 3.6 we apply a convolution quadrature time discretization, based on the Radau IIA Runge–Kutta methods, to the boundary integral equation, which yields a temporally discrete scheme for the approximation of the scattering problem. We introduce some basic results surrounding the convolution quadrature method and crucial notation for the error analysis in the subsequent section, but omit the formulation of semi-discrete error bounds.

Section 3.7 introduces the spatial discretization based on Raviart–Thomas boundary elements and cites the best-approximation result used in this paper. The main part of this section consists of the error analysis, which leads to the main result of Theorem 3.18. Here, the bulk of the previous analysis enters, however the structure of the proof is carried over from [112, Theorem 6.1]. A complication on the way towards pointwise estimates away from the boundary is overcome by requiring additional regularity on the data (by following the ideas of the proof of Lemma 3.2 and (3.53)).

Finally in Section 3.8 we describe the numerical experiments conducted for the present setting. A fractional material law is used with a simple domain to compute empirical convergence rates in space and time, which illustrate the error bounds of the previous sections. An example with two cubes demonstrates the use of the method and closes the paper.

3.2 Reformulation of the problem and mathematical framework

3.2.1 Reformulation of the time-dependent scattering problem

Via the Laplace transforms $(\widehat{\chi}_e^{\pm}(s), \widehat{\chi}_m^{\pm}(s))$ of the susceptibility kernels $(\chi_e^{\pm}(t), \chi_m^{\pm}(t))$, we define the functions

$$\varepsilon^{\pm}(s) = \varepsilon_0(1 + \widehat{\chi}_e^{\pm}(s)), \qquad \mu^{\pm}(s) = \mu_0(1 + \widehat{\chi}_m^{\pm}(s)),$$

which are the Laplace transforms of the distributions $\varepsilon_0(\delta + \chi_e^{\pm})$ and $\mu_0(\delta + \chi_m^{\pm})$ (with Dirac's delta distribution). We use the Heaviside notation for temporal convolution: for a function g defined on the real line,

$$\varepsilon^{\pm}(\partial_t)g = (\mathcal{L}^{-1}\varepsilon^{\pm}) * g, \qquad \mu^{\pm}(\partial_t)g = (\mathcal{L}^{-1}\mu^{\pm}) * g,$$

where $\mathcal{L}^{-1}$ denotes taking the inverse Laplace transform. (We will later use this notation also for temporal convolutions related to other Laplace transforms.) We then arrive at the following reformulation of the scattering problem:

In the interior domain Ω^-:

$$\begin{aligned} \varepsilon^-(\partial_t)\,\partial_t \boldsymbol{E}^- - \mathbf{curl}\,\boldsymbol{H}^- &= 0, \\ \mu^-(\partial_t)\,\partial_t \boldsymbol{H}^- + \mathbf{curl}\,\boldsymbol{E}^- &= 0. \end{aligned}$$

In the exterior domain Ω^+:

$$\begin{aligned} \varepsilon^+(\partial_t)\,\partial_t \boldsymbol{E}^+ - \mathbf{curl}\,\boldsymbol{H}^+ &= 0, \\ \mu^+(\partial_t)\,\partial_t \boldsymbol{H}^+ + \mathbf{curl}\,\boldsymbol{E}^+ &= 0. \end{aligned} \tag{3.7}$$

This is completed by enforcing continuity of the tangential parts of the electromagnetic fields along the boundary, as in (3.6).

3.2.2 Passivity conditions for the dispersive permittivities $\varepsilon^{\pm}(s)$ and permeabilities $\mu^{\pm}(s)$

As is explained in [37, after Definition 2.5], passivity and causality of the time-varying material law result from the following property :

$$\operatorname{Re}\left(\varepsilon^{\pm}(s)s\right) > 0 \quad \text{and} \quad \operatorname{Re}\left(\mu^{\pm}(s)s\right) > 0 \qquad \text{for} \quad \operatorname{Re} s > 0. \tag{3.8}$$

This will be assumed throughout this paper. For our purposes it will sometimes be useful to assume a stronger passivity condition:

$$\operatorname{Re}\left(\varepsilon^{\pm}(s)s\right) \geq \varepsilon_0 \operatorname{Re} s \quad \text{and} \quad \operatorname{Re}\left(\mu^{\pm}(s)s\right) \geq \mu_0 \operatorname{Re} s \qquad \text{for} \quad \operatorname{Re} s > 0. \tag{3.9}$$

This condition is equivalent to $\operatorname{Re}\left(\widehat{\chi}_e^{\pm}(s)s\right) \geq 0$ and $\operatorname{Re}\left(\widehat{\chi}_m^{\pm}(s)s\right) \geq 0$ for $\operatorname{Re} s > 0$.
We further assume a bound for $\varepsilon^{\pm}(s)$ and $\mu^{\pm}(s)$: for every $\sigma > 0$, there exists $M_\sigma < \infty$ such that

$$\left|\varepsilon^{\pm}(s)\right| \leq M_\sigma \varepsilon_0 \quad \text{and} \quad \left|\mu^{\pm}(s)\right| \leq M_\sigma \mu_0 \qquad \text{for} \quad \operatorname{Re} s \geq \sigma > 0. \tag{3.10}$$

Lemma 3.1. *All examples of* (3.5) *satisfy the strong passivity condition* (3.9) *and the bound* (3.10).

Proof. (3.5a) For the Debye model with $\lambda > 0$ and $\beta > 0$ we have, for $\operatorname{Re} s > 0$,

$$\widehat{\chi}_e(s) = (\mathcal{L}\chi_e)(s) = \frac{\beta}{s+\lambda} \quad \text{and hence} \quad \operatorname{Re}\left(\widehat{\chi}_e(s)s\right) = \frac{\beta}{|s+\lambda|^2}\left(|s|^2 + \lambda \operatorname{Re} s\right) \geq 0.$$

More generally, by the same argument we also obtain the strong passivity for completely monotonic susceptibility kernels χ_e.

(3.5b) The Laplace transform of the susceptibility kernel corresponding to the shifted Heaviside function $\chi_e(t) = \alpha_1 + \alpha_2 \Theta(t - t_*)$ reads

$$\widehat{\chi}_e(s) = s^{-1}\left(\alpha_1 + \alpha_2 \mathrm{e}^{-t_* s}\right),$$

for which we obtain the strong passivity under the condition $\alpha_1 \geq \alpha_2$.

(3.5c) The Laplace transform of the susceptibility kernel corresponding to the Drude model reads

$$\widehat{\chi}_e(s) = \frac{\omega_D^2}{s(s+\gamma_D)}, \qquad \text{such that} \qquad \operatorname{Re}\left(\widehat{\chi}_e(s)s\right) = \frac{\omega_D^2}{|s+\gamma_D|^2}\left(\gamma_D + \operatorname{Re} s\right) \geq 0.$$

(3.5d) The Lorentz model is determined by

$$\widehat{\chi}_e(s) = \frac{\beta}{s(s+\alpha)+\omega}, \quad \text{such that} \quad \operatorname{Re}\left(\widehat{\chi}_e(s)s\right) = \frac{\beta}{|s(s+\alpha)+\omega|^2} \operatorname{Re}\left(|s|^2 s + |s|^2 \alpha + s\omega\right) \geq 0.$$

(3.5e) The susceptibility kernel describing the fractional material law is characterized by the Laplace domain function with $\beta > 0, \lambda > 0$ and $0 < \eta < 2$,

$$\widehat{\chi}_e(s) = \frac{\beta}{s^\eta + \lambda}, \quad \text{with} \quad \operatorname{Re}\left(\widehat{\chi}_e(s)s\right) = \frac{\beta\left(\operatorname{Re}\left(s\,\overline{s}^\eta\right) + \lambda \operatorname{Re} s\right)}{|s^\eta + \lambda|^2} = \frac{\beta\left(|s|^{2\eta}\left(\operatorname{Re} s^{1-\eta} + \lambda \operatorname{Re} s\right)\right)}{|s^\eta + \lambda|^2} \geq 0.$$

The bound (3.10) is obvious for each example. □

3.2.3 Temporal convolution

Let $K(s)\colon X \to Y$, for $\operatorname{Re} s > 0$, be an analytic family of bounded linear operators between two Hilbert spaces X and Y. We assume that K is polynomially bounded: there exists a real κ, and for every $\sigma > 0$ there exists $M_\sigma < \infty$, such that

$$\|K(s)\|_{Y \leftarrow X} \le M_\sigma \, |s|^\kappa , \qquad \operatorname{Re} s \ge \sigma > 0. \tag{3.11}$$

This bound ensures that K is the Laplace transform of a distribution of finite order of differentiation with support on the non-negative real half-line $t \ge 0$. For a function $g : [0,T] \to X$, which together with its extension by 0 to the negative real half-line is sufficiently regular, we use the Heaviside operational calculus notation

$$K(\partial_t) g = (\mathcal{L}^{-1} K) * g$$

for the temporal convolution of the inverse Laplace transform of K with g. For the identity operator $\mathrm{Id}(s) = s$, we have $\mathrm{Id}(\partial_t) g = \partial_t g$, the time derivative of g. For two such families of operators $K(s)$ and $L(s)$ mapping into compatible spaces, the associativity of convolution and the product rule of Laplace transforms yield the composition rule

$$K(\partial_t) L(\partial_t) g = (KL)(\partial_t) g. \tag{3.12}$$

For a Hilbert space X, we let $H^r(\mathbb{R}, X)$ be the Sobolev space of order r of X-valued functions on $\mathbb{R}$, and on finite intervals $(0,T)$ we let

$$H_0^r(0,T;X) = \{ g|_{(0,T)} \,:\, g \in H^r(\mathbb{R},X) \;\text{ with }\; g = 0 \;\text{ on }\; (-\infty, 0) \},$$

where the subscript 0 in H_0^r only refers to the left end-point of the interval. For integer $r \ge 0$, the norm $\|\partial_t^r g\|_{L^2(0,T;X)}$ is equivalent to the natural norm on $H_0^r(0,T;X)$. The Plancherel formula yields the following bound [95, Lemma 2.1]: If $K(s)$ is bounded by (3.11) in the half-plane $\operatorname{Re} s > 0$, then $K(\partial_t)$ extends by density to a bounded linear operator $K(\partial_t)$ from $H_0^{r+\kappa}(0,T;X)$ to $H_0^r(0,T;Y)$ with the bound

$$\|K(\partial_t)\|_{H_0^r(0,T;Y) \leftarrow H_0^{r+\kappa}(0,T;X)} \le e M_{1/T}$$

for arbitrary real r. Here the bound on the right-hand side arises from the bound $e^{\sigma T} M_\sigma$ on choosing $\sigma = 1/T$. We note that for any integer $k \ge 0$ and $\alpha > 1/2$, we have the continuous embedding $H_0^{k+\alpha}(0,T;X) \subset C^k([0,T];X)$.

3.2.4 The tangential trace and the trace space $\boldsymbol{X}_\Gamma$

Let Ω be a bounded Lipschitz domain in $\mathbb{R}^3$ with boundary surface $\Gamma = \partial\Omega$ or the complement of the closure of such a domain. For a continuous vector field $\boldsymbol{u} : \overline{\Omega} \to \mathbb{C}^3$, we define the tangential trace

$$\gamma_T \boldsymbol{u} = \boldsymbol{u}|_\Gamma \times \boldsymbol{n} \qquad \text{on } \Gamma,$$

where $\boldsymbol{n}$ denotes the unit surface normal pointing into the exterior domain. We note that the tangential component of $\boldsymbol{u}|_\Gamma$ is $\boldsymbol{u}_T = (\boldsymbol{I} - \boldsymbol{n}\boldsymbol{n}^\top)\boldsymbol{u}|_\Gamma = -(\gamma_T \boldsymbol{u}) \times \boldsymbol{n}$.

By the version of Green's formula for the **curl** operator, we have for sufficiently regular vector fields $\boldsymbol{u}, \mathbf{v} : \overline{\Omega} \to \mathbb{C}^3$ that

$$\int_\Omega \big(\mathbf{curl}\, \boldsymbol{u} \cdot \mathbf{v} - \boldsymbol{u} \cdot \mathbf{curl}\, \mathbf{v} \big) \mathrm{d}x = \int_\Gamma (\gamma_T \boldsymbol{u} \times \boldsymbol{n}) \cdot \gamma_T \mathbf{v} \, \mathrm{d}\sigma,$$

where the dot $\cdot$ stands for the Euclidean inner product on $\mathbb{C}^3$, i.e., $\boldsymbol{a}\cdot\boldsymbol{b}=\overline{\boldsymbol{a}}^\top\boldsymbol{b}$ for $\boldsymbol{a},\boldsymbol{b}\in\mathbb{C}^3$. The right-hand side in this formula defines a skew-hermitian sesquilinear form on continuous tangential vector fields on the boundary, say $\boldsymbol{\phi},\psi:\Gamma\to\mathbb{C}^3$, which we write as

$$[\boldsymbol{\phi},\psi]_\Gamma=\int_\Gamma(\boldsymbol{\phi}\times\boldsymbol{n})\cdot\psi\,\mathrm{d}\sigma.$$

As it was shown in [3] for smooth domains and extended by [30] for Lipschitz domains (see also the survey in [29, Sect. 2.2]), the trace operator γ_T can be extended to a surjective bounded linear operator from the space that appears naturally for Maxwell's equations, $H(\mathbf{curl},\Omega)=\{\mathbf{v}\in\boldsymbol{L}^2(\Omega)\,:\,\mathbf{curl}\,\mathbf{v}\in\boldsymbol{L}^2(\Omega)\}$, to the

$$\text{trace space: a Hilbert space denoted } \mathrm{X}_\Gamma\text{, with norm } \|\cdot\|_{\mathrm{X}_\Gamma}.$$

This space is characterized as the tangential subspace of the Sobolev space $H^{-1/2}(\Gamma)$ with surface divergence in $H^{-1/2}(\Gamma)$ (see the papers cited above for the precise formulation). It has the property that the pairing $[\cdot,\cdot]_\Gamma$ can be extended to a non-degenerate continuous sesquilinear form on $\mathrm{X}_\Gamma\times\mathrm{X}_\Gamma$. With this pairing the space X_Γ becomes its own dual.

3.3 A time-harmonic transmission problem

For the derivation of the parameter-dependent operators and representation formulas we write in this section $\varepsilon(s)$ and $\mu(s)$ either for $\varepsilon^+(s)$ and $\mu^+(s)$ or for $\varepsilon^-(s)$ and $\mu^-(s)$. The single and double layer potentials and the Calderón operator are defined for the same material parameters in the inner and outer domain. In the derivation of the boundary integral equation, this suits the situation, since the solutions of Maxwell's equations are extended to $\mathbb{R}^3\setminus\Gamma$, by setting them to zero on either the inner or outer domain. For notational simplicity, in the proofs we omit the frequency-dependence in the notation.

Formally applying the Laplace transform to Maxwell's equation and inserting the material law (3.2) in (3.1) yields the time-harmonic Maxwell's equations

$$\begin{aligned}\varepsilon(s)s\widehat{\boldsymbol{E}}-\mathbf{curl}\,\widehat{\boldsymbol{H}}&=0\\ \mu(s)s\widehat{\boldsymbol{H}}+\mathbf{curl}\,\widehat{\boldsymbol{E}}&=0\end{aligned}\qquad\text{in }\mathbb{R}^3\setminus\Gamma$$

with the complex-valued analytic functions ε and μ that satisfy the passivity condition (3.8).

3.3.1 Potential operators and representation formulas

The fundamental solution of the time-harmonic Maxwell's equations with $\varepsilon=\mu=1$ reads

$$G(s,x)=\frac{e^{-s|x|}}{4\pi\,|x|},\qquad \operatorname{Re}s>0,\ x\in\mathbb{R}^3\setminus\{0\}.$$

The *electromagnetic single layer potential* operator is denoted by $\boldsymbol{\mathcal{S}}(s)$. Applied to a complex-valued boundary function $\boldsymbol{\varphi}$ of sufficient regularity for the expressions to be finite, and evaluated at a point $x\in\mathbb{R}^3\setminus\Gamma$ away from the boundary, it reads

$$\boldsymbol{\mathcal{S}}(s)\boldsymbol{\varphi}(x)=-s\int_\Gamma G(s,x-y)\boldsymbol{\varphi}(y)\mathrm{d}y+s^{-1}\nabla\int_\Gamma G(s,x-y)\,\mathrm{div}_\Gamma\,\boldsymbol{\varphi}(y)\mathrm{d}y.$$

The *electromagnetic double layer potential* operator is denoted by $\boldsymbol{\mathcal{D}}(s)$ and is given in the same context by

$$\boldsymbol{\mathcal{D}}(s)\boldsymbol{\varphi}(x) = \mathbf{curl} \int_\Gamma G(s, x-y)\boldsymbol{\varphi}(y)\mathrm{d}y.$$

By construction, the potential operators satisfy the relations

$$s\boldsymbol{\mathcal{S}}(s) - \mathbf{curl} \circ \boldsymbol{\mathcal{D}}(s) = 0, \qquad s\boldsymbol{\mathcal{D}}(s) + \mathbf{curl} \circ \boldsymbol{\mathcal{S}}(s) = 0. \tag{3.13}$$

This section relies heavily on electromagnetic transmission problems, formulated on $\mathbb{R}^3 \setminus \Gamma$. Jumps and averages for the tangential traces are defined by

$$[\gamma_T] = \gamma_T^+ - \gamma_T^-, \qquad \{\gamma_T\} = \tfrac{1}{2}\left(\gamma_T^+ + \gamma_T^-\right).$$

The composition of the jumps with the potential operators reveals the *jump relations*

$$[\gamma_T] \circ \boldsymbol{\mathcal{S}}(s) = 0, \qquad [\gamma_T] \circ \boldsymbol{\mathcal{D}}(s) = -\mathbf{Id}. \tag{3.14}$$

For general ε, μ, we use the potential operators

$$\boldsymbol{\mathcal{S}}_{\varepsilon,\mu}(s) = \boldsymbol{\mathcal{S}}\big(s\sqrt{\varepsilon(s)\mu(s)}\big), \quad \boldsymbol{\mathcal{D}}_{\varepsilon,\mu}(s) = \boldsymbol{\mathcal{D}}\big(s\sqrt{\varepsilon(s)\mu(s)}\big). \tag{3.15}$$

The identities (3.13) and the jump relations (3.14) imply that any sufficiently regular boundary densities $(\widehat{\boldsymbol{\varphi}}, \widehat{\boldsymbol{\psi}})$ are associated with electromagnetic fields $(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{H}})$ by

$$\widehat{\boldsymbol{E}} = -\frac{\sqrt{\mu(s)}}{\sqrt{\varepsilon(s)}}\boldsymbol{\mathcal{S}}_{\varepsilon,\mu}(s)\widehat{\boldsymbol{\varphi}} + \boldsymbol{\mathcal{D}}_{\varepsilon,\mu}(s)\widehat{\boldsymbol{\psi}}, \tag{3.16}$$

$$\widehat{\boldsymbol{H}} = -\boldsymbol{\mathcal{D}}_{\varepsilon,\mu}(s)\widehat{\boldsymbol{\varphi}} - \frac{\sqrt{\varepsilon(s)}}{\sqrt{\mu(s)}}\boldsymbol{\mathcal{S}}_{\varepsilon,\mu}(s)\,\widehat{\boldsymbol{\psi}}, \tag{3.17}$$

which solve the transmission problem

$$\varepsilon(s)s\widehat{\boldsymbol{E}} - \mathbf{curl}\,\widehat{\boldsymbol{H}} = 0 \qquad \text{in} \quad \mathbb{R}^3 \setminus \Gamma, \tag{3.18a}$$

$$\mu(s)s\widehat{\boldsymbol{H}} + \mathbf{curl}\,\widehat{\boldsymbol{E}} = 0 \qquad \text{in} \quad \mathbb{R}^3 \setminus \Gamma, \tag{3.18b}$$

$$[\gamma_T]\widehat{\boldsymbol{H}} = \widehat{\boldsymbol{\varphi}}\,, \tag{3.18c}$$

$$-[\gamma_T]\widehat{\boldsymbol{E}} = \widehat{\boldsymbol{\psi}}\,. \tag{3.18d}$$

Up to this point, this section was restricted to the presentation of established operators and identities, which hold for boundary densities of sufficient regularity. The next subsection provides bounds in terms of the appropriate norms, which in particular gives a rigorous setting for the previously defined operators. Before that, we turn to some useful estimates of the terms in formulas (3.15) and (3.16)–(3.17).

The following lemma shows that $\boldsymbol{\mathcal{S}}_{\varepsilon,\mu}(s)$ and $\boldsymbol{\mathcal{D}}_{\varepsilon,\mu}(s)$ behave well for $\operatorname{Re} s > 0$.

Lemma 3.2. *Under the passivity condition* (3.8)*, the argument appearing in the definition of the potential operators* $\boldsymbol{\mathcal{S}}_{\varepsilon,\mu}(s)$ *and* $\boldsymbol{\mathcal{D}}_{\varepsilon,\mu}(s)$ *has positive real part:*

$$\operatorname{Re}\left(s\sqrt{\varepsilon(s)\mu(s)}\right) > 0 \quad \textit{for} \quad \operatorname{Re} s > 0.$$

Under the strong passivity condition (3.9)*, we have with* $c^{-1} = \sqrt{\varepsilon_0\mu_0}$

$$\operatorname{Re}\left(s\sqrt{\varepsilon(s)\mu(s)}\right) \geq c^{-1}\operatorname{Re} s \quad \textit{for} \quad \operatorname{Re} s > 0. \tag{3.19}$$

Proof. We write $\varepsilon(s)s = |\varepsilon(s)s|\, e^{i\varphi_\varepsilon}$ and $\mu(s)s = |\mu(s)s|\, e^{i\varphi_\mu}$, with $\varphi_\mu, \varphi_\varepsilon \in (-\pi/2, \pi/2)$ due to the positivity (3.8). We then have

$$\operatorname{Re}\left(s\sqrt{\varepsilon(s)\mu(s)}\right) = |\varepsilon(s)s|^{1/2}\,|\mu(s)s|^{1/2}\operatorname{Re} e^{i(\varphi_\mu+\varphi_\varepsilon)/2},$$

which is positive since $\operatorname{Re} e^{i(\varphi_\mu+\varphi_\varepsilon)/2} = \cos((\varphi_\mu+\varphi_\varepsilon)/2) > 0$. The inequality (3.19) follows from the general inequality, for $a, b \in \mathbb{C}$ with $\operatorname{Re} a \geq 0$ and $\operatorname{Re} b \geq 0$,

$$\operatorname{Re}\sqrt{ab} \geq \sqrt{\operatorname{Re} a \cdot \operatorname{Re} b}.$$

This inequality is proved using polar coordinates for $a = |a|\, e^{i\alpha}$ and $b = |b|e^{i\beta}$ and the inequalities

$$\cos\left(\tfrac{1}{2}(\alpha+\beta)\right) \geq \tfrac{1}{2}\left(\cos\alpha + \cos\beta\right) \geq \sqrt{\cos\alpha \cdot \cos\beta},$$

where the first inequality results from the concavity of the cosine on $[-\pi/2, \pi/2]$ and the second inequality is the arithmetic-geometric mean inequality. □

In view of (3.16)–(3.17) we further note that under the strong passivity condition (3.9) and the bound (3.10) we have the bounds, for $\operatorname{Re} s \geq \sigma > 0$,

$$\left|\frac{\sqrt{\mu(s)}}{\sqrt{\varepsilon(s)}}\right| = \left|\frac{\sqrt{\mu(s)s}}{\sqrt{\varepsilon(s)s}}\right| \leq \left(\frac{\mu_0\, M_\sigma}{\varepsilon_0}\right)^{1/2} \frac{|s|^{1/2}}{(\operatorname{Re} s)^{1/2}} \quad \text{and} \quad \left|\frac{\sqrt{\varepsilon(s)}}{\sqrt{\mu(s)}}\right| \leq \left(\frac{\varepsilon_0\, M_\sigma}{\mu_0}\right)^{1/2} \frac{|s|^{1/2}}{(\operatorname{Re} s)^{1/2}}. \tag{3.20}$$

3.3.2 Transmission problems and boundary operators

The right-hand side of the representation formula, namely the operator associated to the linear map $(\widehat{\boldsymbol{\varphi}}, \widehat{\boldsymbol{\psi}}) \mapsto (\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{H}})$, extends by density to a bounded linear operator from the trace space ${\mathrm{X}_\Gamma}^2$ to $H(\mathbf{curl}, \Omega)^2$. The following lemma proves this and further provides an s-explicit bound. A related result can be found in [38, Lemma 6.4].

Lemma 3.3. *Let $(\widehat{\boldsymbol{\varphi}}, \widehat{\boldsymbol{\psi}}) \in {\mathrm{X}_\Gamma}^2$ be some complex-valued boundary functions in the trace space. There exist time-harmonic electromagnetic fields $(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{H}})$, that are defined by the representation formulas (3.16)–(3.17), which solve the transmission problem (3.18a)–(3.18d) for $\operatorname{Re} s > 0$ and are bounded by*

$$\left\|\begin{pmatrix}\widehat{\boldsymbol{E}}\\ \widehat{\boldsymbol{H}}\end{pmatrix}\right\|_{H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)^2} \leq C_\Gamma \max\left(\frac{|\varepsilon(s)s|^2+1}{\operatorname{Re}\varepsilon(s)s}, \frac{|\mu(s)s|^2+1}{\operatorname{Re}\mu(s)s}\right)\left\|\begin{pmatrix}\widehat{\boldsymbol{\varphi}}\\ \widehat{\boldsymbol{\psi}}\end{pmatrix}\right\|_{{\mathrm{X}_\Gamma}^2},$$

where the constant $C_\Gamma = \|\{\gamma_T\}\|_{\mathrm{X}_\Gamma \leftarrow H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)}$ is the operator norm of the tangential average trace operator.

Proof. Throughout the proof, we omit the frequency variable s in the material parameters $\varepsilon(s)$ and $\mu(s)$. Green's formula in combination with the time-harmonic Maxwell's equations reads

$$\begin{aligned}\pm\left[\gamma_T^{\pm}\widehat{\boldsymbol{H}}, \gamma_T^{\pm}\widehat{\boldsymbol{E}}\right]_\Gamma &= \int_{\Omega^\pm}\left(\mathbf{curl}\,\widehat{\boldsymbol{H}}\cdot\widehat{\boldsymbol{E}} - \widehat{\boldsymbol{H}}\cdot\mathbf{curl}\,\widehat{\boldsymbol{E}}\right)\mathrm{d}\boldsymbol{x}\\ &= \int_{\Omega^\pm}\left(\bar{\varepsilon}\bar{s}\left|\widehat{\boldsymbol{E}}\right|^2 + \mu s\left|\widehat{\boldsymbol{H}}\right|^2\right)\mathrm{d}\boldsymbol{x}.\end{aligned} \tag{3.21}$$

Recall that Ω^- and Ω^+ refer to the interior and exterior domain, respectively. The conjugation of the Laplace parameter in the first summand stems from the anti-linearity of the inner product, which has been defined via $\boldsymbol{a}\cdot\boldsymbol{b} = \overline{\boldsymbol{a}}^\top\boldsymbol{b}$ on $\mathbb{C}^3$. Summation of these two terms yields the identity

$$\mathrm{I} := \int_{\mathbb{R}^3\setminus\Gamma}\bar{\varepsilon}\bar{s}\left|\widehat{\boldsymbol{E}}\right|^2 + \mu s\left|\widehat{\boldsymbol{H}}\right|^2\mathrm{d}\boldsymbol{x} = \left[\gamma_T^+\widehat{\boldsymbol{H}}, \gamma_T^+\widehat{\boldsymbol{E}}\right]_\Gamma - \left[\gamma_T^-\widehat{\boldsymbol{H}}, \gamma_T^-\widehat{\boldsymbol{E}}\right]_\Gamma. \tag{3.22}$$

Any part of the time-harmonic electromagnetic fields can always be rewritten in terms of each others **curl**, by inserting (3.18a) and (3.18b) respectively. Using the separation $\mathrm{I} = (1-\theta)\mathrm{I} + \theta\mathrm{I}$ and inserting the time-harmonic Maxwell problem in the second summand reformulates the left-hand side to the expression

$$\begin{aligned}\mathrm{I} = \int_{\mathbb{R}^3\setminus\Gamma} \Big(&(1-\theta_1)\bar{\varepsilon}\bar{s}\big|\widehat{\boldsymbol{E}}\big|^2 + \theta_2\mu s\big|(\mu s)^{-1}\,\mathbf{curl}\,\widehat{\boldsymbol{E}}\big|^2 \\ &+ (1-\theta_2)\mu s\big|\widehat{\boldsymbol{H}}\big|^2 + \theta_1\bar{\varepsilon}\bar{s}\big|(\varepsilon s)^{-1}\,\mathbf{curl}\,\widehat{\boldsymbol{H}}\big|^2\Big)\mathrm{d}\boldsymbol{x}.\end{aligned}$$

Taking the real part on both sides slightly simplifies the right-hand side to

$$\begin{aligned}\mathrm{Re}\,\mathrm{I} = \int_{\mathbb{R}^3\setminus\Gamma} \Big(&(1-\theta_1)\mathrm{Re}\,\varepsilon s\big|\widehat{\boldsymbol{E}}\big|^2 + \theta_2\,|\mu s|^{-2}\,\mathrm{Re}\,\mu s\big|\,\mathbf{curl}\,\widehat{\boldsymbol{E}}\big|^2 \\ &+ (1-\theta_2)\mathrm{Re}\,\mu s\big|\widehat{\boldsymbol{H}}\big|^2 + \theta_1\,|\varepsilon s|^{-2}\,\mathrm{Re}\,\varepsilon s\big|\,\mathbf{curl}\,\widehat{\boldsymbol{H}}\big|^2\Big)\mathrm{d}\boldsymbol{x}.\end{aligned}$$

The parameters (θ_1, θ_2) are free and chosen in such a way that the preceding factors of the summands agree, which is achieved by setting $1-\theta_1 = \theta_1|\varepsilon s|^{-2}$ and $1-\theta_2 = \theta_2|\mu s|^{-2}$. Rearranging this requirement leads to the choice of $\theta_1 = 1/(1+|\varepsilon s|^{-2})$and $\theta_2 = 1/(1+|\mu s|^{-2})$. Inserting these particular choices of θ_1 and θ_2 yields the estimate

$$\mathrm{Re}\,\mathrm{I} \geq \min\left(\frac{\mathrm{Re}\,\varepsilon s}{|\varepsilon s|^2+1}, \frac{\mathrm{Re}\,\mu s}{|\mu s|^2+1}\right)\Big(\|\widehat{\boldsymbol{E}}\|^2_{H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)} + \|\widehat{\boldsymbol{H}}\|^2_{H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)}\Big). \tag{3.23}$$

The stated result follows now from following the proof of [112, Lemma 3.1] on from the identity (3.14). To keep the proof self-contained, we conclude with the arguments given there.

The real part of I is, due to the right-hand side of (3.22), also characterized by

$$\mathrm{Re}\,\mathrm{I} = \mathrm{Re}\,\Big(\Big[\gamma_T^+\widehat{\boldsymbol{H}}, \gamma_T^+\widehat{\boldsymbol{E}}\Big]_\Gamma - \Big[\gamma_T^-\widehat{\boldsymbol{H}}, \gamma_T^-\widehat{\boldsymbol{E}}\Big]_\Gamma\Big).$$

Rewriting the right-hand side in terms of jumps and averages bysumming several mixed terms and using the transmission conditions (3.18c)–(3.18d) yields

$$\begin{aligned}\mathrm{Re}\,\mathrm{I} &= \mathrm{Re}\,\Big(\Big[[\gamma_T]\widehat{\boldsymbol{H}}, \{\gamma_T\}\widehat{\boldsymbol{E}}\Big]_\Gamma + \Big[-[\gamma_T]\widehat{\boldsymbol{E}}, \{\gamma_T\}\widehat{\boldsymbol{H}}\Big]_\Gamma\Big) \\ &= \mathrm{Re}\,\Big(\Big[\widehat{\boldsymbol{\varphi}}, \{\gamma_T\}\widehat{\boldsymbol{E}}\Big]_\Gamma + \Big[\widehat{\boldsymbol{\psi}}, \{\gamma_T\}\widehat{\boldsymbol{H}}\Big]_\Gamma\Big).\end{aligned} \tag{3.24}$$

The self-duality of X_Γ implies a Cauchy–Schwarz type inequality with the corresponding norm and the duality pairing $[\cdot,\cdot]_\Gamma$. Combined with the Cauchy–Schwarz inequality on $\mathbb{R}^2$, this yields

$$\begin{aligned}\mathrm{Re}\,\mathrm{I} &\leq \|\widehat{\boldsymbol{\varphi}}\|_{\mathrm{X}_\Gamma}\,\|\{\gamma_T\}\widehat{\boldsymbol{E}}\|_{\mathrm{X}_\Gamma} + \|\widehat{\boldsymbol{\psi}}\|_{\mathrm{X}_\Gamma}\,\|\{\gamma_T\}\widehat{\boldsymbol{H}}\|_{\mathrm{X}_\Gamma} = \begin{pmatrix}\|\widehat{\boldsymbol{\varphi}}\|_{\mathrm{X}_\Gamma}\\ \|\widehat{\boldsymbol{\psi}}\|_{\mathrm{X}_\Gamma}\end{pmatrix}\cdot\begin{pmatrix}\|\{\gamma_T\}\widehat{\boldsymbol{E}}\|_{\mathrm{X}_\Gamma}\\ \|\{\gamma_T\}\widehat{\boldsymbol{H}}\|_{\mathrm{X}_\Gamma}\end{pmatrix} \\ &\leq \Big(\|\widehat{\boldsymbol{\varphi}}\|^2_{\mathrm{X}_\Gamma} + \|\widehat{\boldsymbol{\psi}}\|^2_{\mathrm{X}_\Gamma}\Big)^{1/2}\Big(\|\{\gamma_T\}\widehat{\boldsymbol{E}}\|^2_{\mathrm{X}_\Gamma} + \|\{\gamma_T\}\widehat{\boldsymbol{H}}\|^2_{\mathrm{X}_\Gamma}\Big)^{1/2}.\end{aligned}$$

To estimate the second factor of the above expression, we intend to use the bound of the tangential trace $\{\gamma_T\} : H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma) \to \mathrm{X}_\Gamma$. The time-harmonic electromagnetic fields $\widehat{\boldsymbol{E}}$ and $\widehat{\boldsymbol{H}}$ are in the local Sobolev space $H_{\mathrm{loc}}(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)$ (c.f. [29]). Moreover, the tangential trace $\{\gamma_T\}$ extends to a bounded operator from $H(\mathbf{curl},\Omega_\Gamma)$ to X_Γ, where Ω_Γ is a bounded domain large enough to contain the boundary Γ. Hence, the left-hand side $\mathrm{Re}\,\mathrm{I}$ is bounded and the electromagnetic fields are in the global Sobolev space $H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)$. With the operator norm of the tangential average $C_\Gamma = \|\{\gamma_T\}\|_{\mathrm{X}_\Gamma\leftarrow H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)}$, the right-hand side is therefore bounded via

$$\mathrm{Re}\,\mathrm{I} \leq C_\Gamma\Big(\|\widehat{\boldsymbol{\varphi}}\|^2_{\mathrm{X}_\Gamma} + \|\widehat{\boldsymbol{\psi}}\|^2_{\mathrm{X}_\Gamma}\Big)^{1/2}\Big(\|\widehat{\boldsymbol{E}}\|^2_{H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)} + \|\widehat{\boldsymbol{H}}\|^2_{H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)}\Big)^{1/2}.$$

Inserting (3.23) on the left-hand side and dividing through the second factor on the right-hand side yields the stated bound. □

In both the time-dependent and time-harmonic situation, our approach consists of determining the tangential traces of the Maxwell solutions by the respective boundary integral equation, and inserting these into the representation formulas to obtain the electromagnetic fields. In this situation, the boundary densities reduce to the tangential traces of the interior and exterior fields respectively, which is a setting that enables an improvement of the bound described in Lemma 3.3. The following Lemma gives these improved bounds.

Lemma 3.4. *In the situation of Lemma 3.3 further assume that the interior (exterior) tangential traces of* $\widehat{\boldsymbol{E}}$ *and* $\widehat{\boldsymbol{H}}$ *are identically* 0*, which implies* $\gamma_T^- \widehat{\boldsymbol{H}} = \widehat{\boldsymbol{\varphi}}$ *(*$-\gamma_T^+ \widehat{\boldsymbol{H}} = \widehat{\boldsymbol{\varphi}}$*) and* $-\gamma_T^- \widehat{\boldsymbol{E}} = \widehat{\boldsymbol{\psi}}$ *(*$\gamma_T^+ \widehat{\boldsymbol{E}} = \widehat{\boldsymbol{\psi}}$*). Then, the bound of Lemma 3.3 improves to*

$$\left\| \begin{pmatrix} \widehat{\boldsymbol{E}} \\ \widehat{\boldsymbol{H}} \end{pmatrix} \right\|_{H(\mathbf{curl},\Omega^\pm)^2} \leq \frac{1}{\sqrt{2}} \left(\max \left(\frac{|\varepsilon(s)s|^2+1}{\operatorname{Re}\varepsilon(s)s}, \frac{|\mu(s)s|^2+1}{\operatorname{Re}\mu(s)s} \right) \right)^{1/2} \left\| \begin{pmatrix} \widehat{\boldsymbol{\varphi}} \\ \widehat{\boldsymbol{\psi}} \end{pmatrix} \right\|_{\mathrm{X}_\Gamma{}^2}.$$

Furthermore, we have the L^2*-bound*

$$\left\| \begin{pmatrix} \widehat{\boldsymbol{E}} \\ \widehat{\boldsymbol{H}} \end{pmatrix} \right\|_{L^2(\Omega^\pm)^2} \leq \frac{1}{\sqrt{2}} \left(\max \left(\frac{1}{\operatorname{Re}\varepsilon(s)s}, \frac{1}{\operatorname{Re}\mu(s)s} \right) \right)^{1/2} \left\| \begin{pmatrix} \widehat{\boldsymbol{\varphi}} \\ \widehat{\boldsymbol{\psi}} \end{pmatrix} \right\|_{\mathrm{X}_\Gamma{}^2}.$$

Proof. The proof of the $H(\mathbf{curl},\Omega^\pm)$ bound is identical to that of Lemma 3.3 down to (3.24), which now implies the bound $\operatorname{Re} I \leq \frac{1}{2}\big(\|\widehat{\boldsymbol{\varphi}}\|_{\mathrm{X}_\Gamma}^2 + \|\widehat{\boldsymbol{\psi}}\|_{\mathrm{X}_\Gamma}^2 \big)$ and yields the stated result. The proof of the L^2-bound is even simpler, working directly with (3.22) instead of (3.23). □

3.3.3 Time-harmonic boundary integral operators and the Calderón operator

The composition of the tangential averages with the potential operators defines the electromagnetic *single and double layer boundary operators*, which operate on the trace space X_Γ and are defined as

$$\boldsymbol{V}_{\varepsilon,\mu}(s) = \{\gamma_T\} \circ \boldsymbol{\mathcal{S}}_{\varepsilon,\mu}(s), \qquad \boldsymbol{K}_{\varepsilon,\mu}(s) = \{\gamma_T\} \circ \boldsymbol{\mathcal{D}}_{\varepsilon,\mu}(s).$$

The *Calderón operator* is a block operator consisting of these boundary operators and has, with a different scaling with respect to the magnetic permeability, been introduced in the dielectric setting (i.e. real-valued and positive ε and μ) by [84] (note the sign correction from [110]). In the present setting we obtain the following Calderón operator, which reads

$$\boldsymbol{C}_{\varepsilon,\mu}(s) = \begin{pmatrix} -\frac{\sqrt{\mu(s)}}{\sqrt{\varepsilon(s)}} \boldsymbol{V}_{\varepsilon,\mu}(s) & \boldsymbol{K}_{\varepsilon,\mu}(s) \\ -\boldsymbol{K}_{\varepsilon,\mu}(s) & -\frac{\sqrt{\varepsilon(s)}}{\sqrt{\mu(s)}} \boldsymbol{V}_{\varepsilon,\mu}(s) \end{pmatrix}, \tag{3.25}$$

where the form of the block operator on the right originates in the representation formula (3.16)–(3.17). Consider outgoing solutions of the time-harmonic Maxwell's equations $\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{H}}$, thus characterized by the representation formulas. The composition of the tangential averages with the representation formulas reveals the jump relations of the Calderón operator (see (3.18a)–(3.18d)):

$$\boldsymbol{C}_{\varepsilon,\mu}(s) \begin{pmatrix} [\gamma_T]\widehat{\boldsymbol{H}} \\ -[\gamma_T]\widehat{\boldsymbol{E}} \end{pmatrix} = \begin{pmatrix} \{\gamma_T\}\widehat{\boldsymbol{E}} \\ \{\gamma_T\}\widehat{\boldsymbol{H}} \end{pmatrix}. \tag{3.26}$$

The application of this operator is thus equivalent to transform jumps of the transmission problem to averages, which directly implies bounds from above through Lemma 3.3.

As a direct consequence, we obtain the following bound, equivalent to [112, Lemma 3.4] in the dielectric case. Earlier, slightly different bounds can be found in the dielectric case in [9, Theorem 4.4] and [84, Lemma 2.3], which are of the order $O(|s|^2)$.

Lemma 3.5. *For s with positive real part, the Calderón operator is a linear operator family on the trace space $\boldsymbol{C}_{\varepsilon,\mu}(s) : {\mathrm{X}_\Gamma}^2 \to {\mathrm{X}_\Gamma}^2$ and satisfies the bound*

$$\|\boldsymbol{C}_{\varepsilon,\mu}(s)\|_{{\mathrm{X}_\Gamma}^2 \leftarrow {\mathrm{X}_\Gamma}^2} \leq C_\Gamma \max\left(\frac{|\varepsilon(s)s|^2+1}{\operatorname{Re}\varepsilon(s)s}, \frac{|\mu(s)s|^2+1}{\operatorname{Re}\mu(s)s}\right),$$

where again $C_\Gamma = \|\{\gamma_T\}\|_{\mathrm{X}_\Gamma \leftarrow H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)}$. The identical bound holds for the components of the Calderón operator (3.25) and for the electromagnetic single and double layer boundary operators $\boldsymbol{V}_{\varepsilon,\mu}(s)$ and $\boldsymbol{K}_{\varepsilon,\mu}(s)$.

The skew-hermitian pairing $[\cdot,\cdot]_\Gamma$ is notationally extended from $\mathrm{X}_\Gamma \times \mathrm{X}_\Gamma$ to ${\mathrm{X}_\Gamma}^2 \times {\mathrm{X}_\Gamma}^2$ in the natural way:

$$\left[\begin{pmatrix}\boldsymbol{\varphi}\\ \psi\end{pmatrix}, \begin{pmatrix}\boldsymbol{\upsilon}\\ \boldsymbol{\xi}\end{pmatrix}\right]_\Gamma = [\boldsymbol{\varphi},\boldsymbol{\upsilon}]_\Gamma + [\psi,\boldsymbol{\xi}]_\Gamma.$$

As was shown in [84, Lemma 3.1] in the dielectric case with positive and real-valued ε and μ, the Calderón operator $\boldsymbol{C}(s)$ is positive with respect to this extended skew-symmetric pairing $[\cdot,\cdot]_\Gamma$. The following lemma transfers this key property to the present setting of analytic $\varepsilon(s)$ and $\mu(s)$.

Lemma 3.6. *The Calderón operator is of positive type: For $\operatorname{Re} s > 0$,*

$$\operatorname{Re}\left[\begin{pmatrix}\boldsymbol{\varphi}\\ \psi\end{pmatrix}, \boldsymbol{C}_{\varepsilon,\mu}(s)\begin{pmatrix}\boldsymbol{\varphi}\\ \psi\end{pmatrix}\right]_\Gamma \geq c_\Gamma^{-2} \min\left(\frac{\operatorname{Re}\varepsilon(s)s}{|\varepsilon(s)s|^2+1}, \frac{\operatorname{Re}\mu(s)s}{|\mu(s)s|^2+1}\right)\left(\|\boldsymbol{\varphi}\|^2_{\mathrm{X}_\Gamma} + \|\psi\|^2_{\mathrm{X}_\Gamma}\right)$$

for all $(\boldsymbol{\varphi},\psi) \in {\mathrm{X}_\Gamma}^2$. The constant is the norm of the jump operator associated to the tangential trace, i.e. $c_\Gamma = \|[\gamma_T]\|_{\mathrm{X}_\Gamma \leftarrow H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)}$.

Proof. Consider $(\widehat{\boldsymbol{\varphi}},\widehat{\boldsymbol{\psi}}) \in {\mathrm{X}_\Gamma}^2$ and let the time-harmonic fields $\widehat{\boldsymbol{E}},\widehat{\boldsymbol{H}} \in H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)$ be given through the representation formula, therefore solving the associated transmission problem of Lemma 3.3. The result is then given by the following chain of inequalities, taken from the proof of [112, Lemma 3.5]

$$\begin{aligned}
&\left\|\begin{pmatrix}\widehat{\boldsymbol{\varphi}}\\ \widehat{\boldsymbol{\psi}}\end{pmatrix}\right\|^2_{\mathrm{X}_\Gamma\times\mathrm{X}_\Gamma} = \left\|\begin{pmatrix}[\gamma_T]\widehat{\boldsymbol{H}}\\ -[\gamma_T]\widehat{\boldsymbol{E}}\end{pmatrix}\right\|^2_{\mathrm{X}_\Gamma\times\mathrm{X}_\Gamma} && \text{by (3.18c)–(3.18d)}\\
&\leq c_\Gamma^2\left(\|\widehat{\boldsymbol{H}}\|^2_{H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)} + \|\widehat{\boldsymbol{E}}\|^2_{H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)}\right) && \text{by def. of } c_\Gamma\\
&\leq c_\Gamma^2 \max\left(\frac{|\varepsilon s|^2+1}{\operatorname{Re}\varepsilon s}, \frac{|\mu s|^2+1}{\operatorname{Re}\mu s}\right)\operatorname{Re}\left[\begin{pmatrix}[\gamma_T]\widehat{\boldsymbol{H}}\\ -[\gamma_T]\widehat{\boldsymbol{E}}\end{pmatrix}, \begin{pmatrix}\{\gamma_T\}\widehat{\boldsymbol{E}}\\ \{\gamma_T\}\widehat{\boldsymbol{H}}\end{pmatrix}\right]_\Gamma && \text{by (3.23)–(3.24)}\\
&= c_\Gamma^2 \max\left(\frac{|\varepsilon s|^2+1}{\operatorname{Re}\varepsilon s}, \frac{|\mu s|^2+1}{\operatorname{Re}\mu s}\right)\operatorname{Re}\left[\begin{pmatrix}[\gamma_T]\widehat{\boldsymbol{H}}\\ -[\gamma_T]\widehat{\boldsymbol{E}}\end{pmatrix}, \boldsymbol{C}_{\varepsilon,\mu}(s)\begin{pmatrix}[\gamma_T]\widehat{\boldsymbol{H}}\\ -[\gamma_T]\widehat{\boldsymbol{E}}\end{pmatrix}\right]_\Gamma && \text{by (3.26)}\\
&= c_\Gamma^2 \max\left(\frac{|\varepsilon s|^2+1}{\operatorname{Re}\varepsilon s}, \frac{|\mu s|^2+1}{\operatorname{Re}\mu s}\right)\operatorname{Re}\left[\begin{pmatrix}\widehat{\boldsymbol{\varphi}}\\ \widehat{\boldsymbol{\psi}}\end{pmatrix}, \boldsymbol{C}_{\varepsilon,\mu}(s)\begin{pmatrix}\widehat{\boldsymbol{\varphi}}\\ \widehat{\boldsymbol{\psi}}\end{pmatrix}\right]_\Gamma && \text{by (3.18c)–(3.18d).}
\end{aligned}$$

□

3.4 The time-harmonic scattering problem

The time-harmonic problem formulation reads

$$\begin{aligned} \varepsilon^{\pm}(s)s\widehat{\boldsymbol{E}}^{\pm} - \mathbf{curl}\,\widehat{\boldsymbol{H}}^{\pm} &= 0 \\ \mu^{\pm}(s)s\widehat{\boldsymbol{H}}^{\pm} + \mathbf{curl}\,\widehat{\boldsymbol{E}}^{\pm} &= 0 \end{aligned} \qquad \text{in } \Omega^{\pm}, \tag{3.27}$$

completed by the transmission conditions, which enforce the continuity of the time-harmonic electromagnetic fields $\widehat{\boldsymbol{E}}$ and $\widehat{\boldsymbol{H}}$:

$$\begin{aligned} \gamma_T\widehat{\boldsymbol{E}}^{+} + \gamma_T\widehat{\boldsymbol{E}}^{+}_{\mathrm{inc}} &= \gamma_T\widehat{\boldsymbol{E}}^{-} \\ \gamma_T\widehat{\boldsymbol{H}}^{+} + \gamma_T\widehat{\boldsymbol{H}}^{+}_{\mathrm{inc}} &= \gamma_T\widehat{\boldsymbol{H}}^{-} \end{aligned} \qquad \text{on } \Gamma. \tag{3.28}$$

3.4.1 The time-harmonic boundary integral equation

In this subsection we derive the time-harmonic boundary integral equation, which determines the boundary densities to be inserted into the representation formulas for the electromagnetic fields. Assuming that we are given solutions to the time-harmonic Maxwell's equations in the exterior or interior domain $\Omega^{\pm}$, we obtain solutions on $\mathbb{R}^3 \setminus \Gamma$ by extension to zero on $\Omega^{\mp}$. Then, jumps and averages reduce to outer or inner traces, respectively. We start by collecting the (supposed) solutions of the boundary integral equations in the vectors

$$\widehat{\boldsymbol{\phi}}^{+} = \begin{pmatrix} \widehat{\boldsymbol{\varphi}}^{+} \\ \widehat{\boldsymbol{\psi}}^{+} \end{pmatrix} = \begin{pmatrix} \gamma_T^{+}\widehat{\boldsymbol{H}}^{+} \\ -\gamma_T^{+}\widehat{\boldsymbol{E}}^{+} \end{pmatrix}, \qquad \widehat{\boldsymbol{\phi}}^{-} = \begin{pmatrix} \widehat{\boldsymbol{\varphi}}^{-} \\ \widehat{\boldsymbol{\psi}}^{-} \end{pmatrix} = \begin{pmatrix} -\gamma_T^{-}\widehat{\boldsymbol{H}}^{-} \\ \gamma_T^{-}\widehat{\boldsymbol{E}}^{-} \end{pmatrix},$$

and denote the block operator $\boldsymbol{J}$ and the trace of the incoming wave $\widehat{\boldsymbol{g}}^{\mathrm{inc}}$ by

$$\boldsymbol{J} = \frac{1}{2}\begin{pmatrix} & -\mathbf{Id} \\ \mathbf{Id} & \end{pmatrix}, \qquad \widehat{\boldsymbol{g}}^{\mathrm{inc}} = \frac{1}{2}\begin{pmatrix} \gamma_T^{+}\widehat{\boldsymbol{E}}^{+}_{\mathrm{inc}} \\ \gamma_T^{+}\widehat{\boldsymbol{H}}^{+}_{\mathrm{inc}} \end{pmatrix}.$$

In order to derive the boundary integral equation, we first use (3.26), followed by the transmission conditions (3.28). This yields

$$\boldsymbol{C}_{\varepsilon^{+},\mu^{+}}(s)\widehat{\boldsymbol{\phi}}^{+} = \frac{1}{2}\begin{pmatrix} \gamma_T^{+}\widehat{\boldsymbol{E}}^{+} \\ \gamma_T^{+}\widehat{\boldsymbol{H}}^{+} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \gamma_T^{-}\widehat{\boldsymbol{E}}^{-} \\ \gamma_T^{-}\widehat{\boldsymbol{H}}^{-} \end{pmatrix} - \widehat{\boldsymbol{g}}^{\mathrm{inc}} = -\boldsymbol{J}\widehat{\boldsymbol{\phi}}^{-} - \widehat{\boldsymbol{g}}^{\mathrm{inc}},$$

and

$$\boldsymbol{C}_{\varepsilon^{-},\mu^{-}}(s)\widehat{\boldsymbol{\phi}}^{-} = \frac{1}{2}\begin{pmatrix} \gamma_T^{-}\widehat{\boldsymbol{E}}^{-} \\ \gamma_T^{-}\widehat{\boldsymbol{H}}^{-} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \gamma_T^{+}\widehat{\boldsymbol{E}}^{+} \\ \gamma_T^{+}\widehat{\boldsymbol{H}}^{+} \end{pmatrix} - \widehat{\boldsymbol{g}}^{\mathrm{inc}} = \boldsymbol{J}\widehat{\boldsymbol{\phi}}^{+} + \widehat{\boldsymbol{g}}^{\mathrm{inc}}.$$

Introducing the family of operators $\boldsymbol{A}(s) : {\mathrm{X}_{\Gamma}}^4 \to {\mathrm{X}_{\Gamma}}^4$ defined as

$$\boldsymbol{A}(s) \coloneqq \begin{pmatrix} \boldsymbol{C}_{\varepsilon^{+},\mu^{+}}(s) & \boldsymbol{J} \\ -\boldsymbol{J} & \boldsymbol{C}_{\varepsilon^{-},\mu^{-}}(s) \end{pmatrix},$$

we arrive at the time-harmonic boundary integral equation

$$\boldsymbol{A}(s)\begin{pmatrix} \widehat{\boldsymbol{\phi}}^{+} \\ \widehat{\boldsymbol{\phi}}^{-} \end{pmatrix} = \begin{pmatrix} -\widehat{\boldsymbol{g}}^{\mathrm{inc}} \\ \widehat{\boldsymbol{g}}^{\mathrm{inc}} \end{pmatrix}. \tag{3.29}$$

This boundary integral equation will be considered in its weak formulation: For $\operatorname{Re} s > 0$ and given $\widehat{\boldsymbol{g}}^{\mathrm{inc}} \in {\mathrm{X}_\Gamma}^2$, find $(\boldsymbol{\phi}^+, \boldsymbol{\phi}^-) \in {\mathrm{X}_\Gamma}^4$ such that, for all $(\boldsymbol{\upsilon}, \boldsymbol{\xi}) \in {\mathrm{X}_\Gamma}^4$

$$\left[\begin{pmatrix} \boldsymbol{\upsilon} \\ \boldsymbol{\xi} \end{pmatrix}, \boldsymbol{A}(s) \begin{pmatrix} \boldsymbol{\phi}^+ \\ \boldsymbol{\phi}^- \end{pmatrix} \right]_\Gamma = \left[\begin{pmatrix} \boldsymbol{\upsilon} \\ \boldsymbol{\xi} \end{pmatrix}, \begin{pmatrix} -\widehat{\boldsymbol{g}}^{\mathrm{inc}} \\ \widehat{\boldsymbol{g}}^{\mathrm{inc}} \end{pmatrix} \right]_\Gamma . \tag{3.30}$$

Crucially, the bilinear form on the left-hand side is coercive, as will be shown next.

3.4.2 Well-posedness of the boundary integral equation

This section is dedicated to the well-posedness of the time-harmonic boundary integral equation, which is shown by employing the Lax-Milgram Lemma. To simplify the expressions in this section, we use the abbreviation

$$m_{\varepsilon,\mu}(s) \coloneqq \max\left(\frac{|\varepsilon^+(s)s|^2+1}{\operatorname{Re}\varepsilon^+(s)s}, \frac{|\mu^+(s)s|^2+1}{\operatorname{Re}\mu^+(s)s}, \frac{|\varepsilon^-(s)s|^2+1}{\operatorname{Re}\varepsilon^-(s)s}, \frac{|\mu^-(s)s|^2+1}{\operatorname{Re}\mu^-(s)s} \right). \tag{3.31}$$

Under the strong passivity condition (3.9) there is a convenient upper bound for $m_{\varepsilon,\mu}(s)$: (3.9)–(3.10) imply that for every $\sigma > 0$ there exists $C_\sigma < \infty$ such that

$$m_{\varepsilon,\mu}(s) \leq C_\sigma \frac{|s|^2}{\operatorname{Re} s} \quad \text{for} \quad \operatorname{Re} s \geq \sigma.$$

We start by giving a bound for the boundary integral operator.

Lemma 3.7. *The analytic operator family $\boldsymbol{A}(s)\colon {\mathrm{X}_\Gamma}^4 \leftarrow {\mathrm{X}_\Gamma}^4$ satisfies, for $\operatorname{Re} s > 0$, the bound*

$$\|\boldsymbol{A}(s)\|_{{\mathrm{X}_\Gamma}^4 \leftarrow {\mathrm{X}_\Gamma}^4} \leq C_\Gamma\, m_{\varepsilon,\mu}(s) + \frac{1}{2},$$

where $C_\Gamma = \|\{\gamma_T\}\|_{\mathrm{X}_\Gamma \leftarrow H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)}$.

Moreover, we have the following coercivity result for the integral operator corresponding to the boundary integral equation.

Lemma 3.8. *The operator family $\boldsymbol{A}(s)$ satisfies the following coercivity property: for $\operatorname{Re} s > 0$ we have the bound*

$$\operatorname{Re}\left[\begin{pmatrix} \boldsymbol{\phi}^+ \\ \boldsymbol{\phi}^- \end{pmatrix}, \boldsymbol{A}(s) \begin{pmatrix} \boldsymbol{\phi}^+ \\ \boldsymbol{\phi}^- \end{pmatrix} \right]_\Gamma \geq c_\Gamma^{-2} m_{\varepsilon,\mu}(s)^{-1} \left(\|\boldsymbol{\phi}^+\|^2_{{\mathrm{X}_\Gamma}^2} + \|\boldsymbol{\phi}^-\|^2_{{\mathrm{X}_\Gamma}^2} \right),$$

for all $(\boldsymbol{\phi}^+, \boldsymbol{\phi}^-) \in {\mathrm{X}_\Gamma}^2 \times {\mathrm{X}_\Gamma}^2$, where $c_\Gamma = \|[\gamma_T]\|_{\mathrm{X}_\Gamma \leftarrow H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)}$.

Proof. We split the operator in the pairing

$$\begin{aligned} \operatorname{Re}\left[\begin{pmatrix} \boldsymbol{\phi}^+ \\ \boldsymbol{\phi}^- \end{pmatrix}, \boldsymbol{A}(s) \begin{pmatrix} \boldsymbol{\phi}^+ \\ \boldsymbol{\phi}^- \end{pmatrix} \right]_\Gamma &= \operatorname{Re}\left[\begin{pmatrix} \boldsymbol{\phi}^+ \\ \boldsymbol{\phi}^- \end{pmatrix}, \begin{pmatrix} \boldsymbol{C}_{\varepsilon^+,\mu^+}(s) & \\ & \boldsymbol{C}_{\varepsilon^-,\mu^-}(s) \end{pmatrix} \begin{pmatrix} \boldsymbol{\phi}^+ \\ \boldsymbol{\phi}^- \end{pmatrix} \right]_\Gamma \\ &\quad + \operatorname{Re}\left[\begin{pmatrix} \boldsymbol{\phi}^+ \\ \boldsymbol{\phi}^- \end{pmatrix}, \begin{pmatrix} & \boldsymbol{J} \\ -\boldsymbol{J} & \end{pmatrix} \begin{pmatrix} \boldsymbol{\phi}^+ \\ \boldsymbol{\phi}^- \end{pmatrix} \right]_\Gamma, \end{aligned}$$

where the first summand is bounded from below by the coercivity of the Calderón operators given in Lemma 3.6. The second summand vanishes due to symmetry of $\boldsymbol{J}$, which we verify next. We have

$$2\operatorname{Re}\left[\widetilde{\boldsymbol{\phi}}, \boldsymbol{J}\boldsymbol{\phi} \right]_\Gamma = \operatorname{Re}\left[\boldsymbol{\phi}_1, -\widetilde{\boldsymbol{\phi}}_2 \right]_\Gamma + \operatorname{Re}\left[\boldsymbol{\phi}_2, \widetilde{\boldsymbol{\phi}}_1 \right]_\Gamma = 2\operatorname{Re}\left[\boldsymbol{\phi}, \boldsymbol{J}\widetilde{\boldsymbol{\phi}} \right]_\Gamma,$$

and therefore,

$$\operatorname{Re}\left[\begin{pmatrix}\boldsymbol{\phi}^+\\ \boldsymbol{\phi}^-\end{pmatrix}, \begin{pmatrix} & \boldsymbol{J}\\ -\boldsymbol{J} & \end{pmatrix}\begin{pmatrix}\boldsymbol{\phi}^+\\ \boldsymbol{\phi}^-\end{pmatrix}\right]_\Gamma = \operatorname{Re}\left[\boldsymbol{\phi}^+, \boldsymbol{J}\boldsymbol{\phi}^-\right]_\Gamma - \operatorname{Re}\left[\boldsymbol{\phi}^-, \boldsymbol{J}\boldsymbol{\phi}^+\right]_\Gamma = 0,$$

such that the claim follows. □

In view of this coercivity, we obtain the following wellposedness result.

Proposition 3.9 (Well-posedness of the time-harmonic boundary integral equation)**.** *Consider the boundary integral equation* (3.29) *for* $\operatorname{Re} s > 0$*. The boundary integral equation has a unique solution*

$$\begin{pmatrix}\widehat{\boldsymbol{\phi}}^+\\ \widehat{\boldsymbol{\phi}}^-\end{pmatrix} = \boldsymbol{A}(s)^{-1}\begin{pmatrix}-\widehat{\boldsymbol{g}}^{\mathrm{inc}}\\ \widehat{\boldsymbol{g}}^{\mathrm{inc}}\end{pmatrix} \in \mathrm{X}_\Gamma{}^4,$$

which satisfies

$$\left\|\begin{pmatrix}\widehat{\boldsymbol{\phi}}^+\\ \widehat{\boldsymbol{\phi}}^-\end{pmatrix}\right\|_{\mathrm{X}_\Gamma{}^4} \leq c_\Gamma^2\, m_{\varepsilon,\mu}(s)\,\sqrt{2}\,\left\|\widehat{\boldsymbol{g}}^{\mathrm{inc}}\right\|_{\mathrm{X}_\Gamma{}^2}.$$

The constant c_Γ *is again the norm of the tangential jump operator, and* $m_{\varepsilon,\mu}(s)$ *is defined in* (3.31)*.*

Proof. The statement follows directly from the Lax–Milgram lemma with the coercivity of Lemma 3.8. □

Using the above properties, we prove the following result, where the domain Ω stands for either Ω^+ or Ω^-.

Proposition 3.10 (Well-posedness of the time-harmonic scattering problem)**.** *For* $\operatorname{Re} s > 0$ *there exists a unique solution* $(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{H}}) \in H(\mathbf{curl}, \mathbb{R}^3\setminus\Gamma) \times H(\mathbf{curl}, \mathbb{R}^3\setminus\Gamma)$ *to the time-harmonic transmission problem* (3.27)–(3.28)*. This solution is characterized by the representation formulas* (3.16)–(3.17)*, where the tangential traces are given by the unique solution of the boundary integral equation* (3.29) *via*

$$\widehat{\boldsymbol{\phi}}^+ = \begin{pmatrix}\gamma_T^+\widehat{\boldsymbol{H}}^+\\ -\gamma_T^+\widehat{\boldsymbol{E}}^+\end{pmatrix}, \qquad \widehat{\boldsymbol{\phi}}^- = \begin{pmatrix}-\gamma_T^-\widehat{\boldsymbol{H}}^-\\ \gamma_T^-\widehat{\boldsymbol{E}}^-\end{pmatrix}.$$

The scattered electromagnetic fields are bounded by

$$\left\|\begin{pmatrix}\widehat{\boldsymbol{E}}\\ \widehat{\boldsymbol{H}}\end{pmatrix}\right\|_{H(\mathbf{curl},\mathbb{R}^3\setminus\Gamma)^2} \leq C_\Gamma\left(m_{\varepsilon,\mu}(s)\right)^{3/2}\left\|\widehat{\boldsymbol{g}}^{\mathrm{inc}}\right\|_{\mathrm{X}_\Gamma{}^2}. \tag{3.32}$$

Proof. Let $(\widehat{\boldsymbol{\varphi}}^+, \widehat{\boldsymbol{\psi}}^+, \widehat{\boldsymbol{\varphi}}^-, \widehat{\boldsymbol{\psi}}^-)$ be the solution of the time-harmonic boundary integral equation (3.29). We insert the boundary densities into the representation formulas and obtain electromagnetic fields $(\widehat{\boldsymbol{E}}^+, \widehat{\boldsymbol{E}}^-, \widehat{\boldsymbol{H}}^+, \widehat{\boldsymbol{H}}^-)$, each defined on $\mathbb{R}^3\setminus\Gamma$, such that

$$\widehat{\boldsymbol{\phi}}^+ = \begin{pmatrix}\widehat{\boldsymbol{\varphi}}^+\\ \widehat{\boldsymbol{\psi}}^+\end{pmatrix} = \begin{pmatrix}[\gamma_T]\widehat{\boldsymbol{H}}^+\\ -[\gamma_T]\widehat{\boldsymbol{E}}^+\end{pmatrix} \quad \text{and} \quad \widehat{\boldsymbol{\phi}}^- = \begin{pmatrix}\widehat{\boldsymbol{\varphi}}^-\\ \widehat{\boldsymbol{\psi}}^-\end{pmatrix} = \begin{pmatrix}[\gamma_T]\widehat{\boldsymbol{H}}^-\\ -[\gamma_T]\widehat{\boldsymbol{E}}^-\end{pmatrix}.$$

The first two components of the left-hand side of boundary integral equation read

$$-\widehat{\boldsymbol{g}}^{\mathrm{inc}} = \boldsymbol{C}_{\varepsilon^+,\mu^+}(s)\widehat{\boldsymbol{\phi}}^+ + \boldsymbol{J}\widehat{\boldsymbol{\phi}}^- = \begin{pmatrix}\{\gamma_T\}\widehat{\boldsymbol{E}}^+\\ \{\gamma_T\}\widehat{\boldsymbol{H}}^+\end{pmatrix} + \frac{1}{2}\begin{pmatrix}[\gamma_T]\widehat{\boldsymbol{E}}^-\\ [\gamma_T]\widehat{\boldsymbol{H}}^-\end{pmatrix} \tag{3.33}$$

and the last two read

$$\widehat{\boldsymbol{g}}^{\mathrm{inc}} = -\boldsymbol{J}\widehat{\boldsymbol{\phi}}^{+} + \boldsymbol{C}_{\varepsilon^-,\mu^-}(s)\widehat{\boldsymbol{\phi}}^{-} = \frac{1}{2}\begin{pmatrix} -[\gamma_T]\widehat{\boldsymbol{E}}^{+} \\ -[\gamma_T]\widehat{\boldsymbol{H}}^{+} \end{pmatrix} + \begin{pmatrix} \{\gamma_T\}\widehat{\boldsymbol{E}}^{-} \\ \{\gamma_T\}\widehat{\boldsymbol{H}}^{-} \end{pmatrix}. \tag{3.34}$$

Subtraction of these components yields precisely the transmission conditions (3.6), namely

$$\begin{pmatrix} \gamma_T^+\widehat{\boldsymbol{E}}^{+}_{\mathrm{inc}} \\ \gamma_T^+\widehat{\boldsymbol{H}}^{+}_{\mathrm{inc}} \end{pmatrix} = \begin{pmatrix} -\gamma_T^+\widehat{\boldsymbol{E}}^{+} + \gamma_T^-\widehat{\boldsymbol{E}}^{-} \\ -\gamma_T^+\widehat{\boldsymbol{H}}^{+} + \gamma_T^-\widehat{\boldsymbol{H}}^{-} \end{pmatrix}.$$

The fields $(\widehat{\boldsymbol{E}}^{+}, \widehat{\boldsymbol{H}}^{+})|_{\Omega^+}$ and $(\widehat{\boldsymbol{E}}^{-}, \widehat{\boldsymbol{H}}^{-})|_{\Omega^-}$ therefore uniquely solve the transmission problem of interest.

Summation of the components (3.33)–(3.34) yields conversely

$$\begin{pmatrix} \gamma_T^-\widehat{\boldsymbol{E}}^{+} + \gamma_T^+\widehat{\boldsymbol{E}}^{-} \\ \gamma_T^-\widehat{\boldsymbol{H}}^{+} + \gamma_T^+\widehat{\boldsymbol{H}}^{-} \end{pmatrix} = 0.$$

In the following, we test these equations via the anti-symmetric pairing and specific test functions. Inserting the test function $\gamma_T^-\widehat{\boldsymbol{H}}^{+}$ in the first component and $\gamma_T^+\widehat{\boldsymbol{E}}^{-}$ in the second component yields

$$\begin{aligned} 0 &= \mathrm{Re}\left[\gamma_T^-\widehat{\boldsymbol{H}}^{+}, \gamma_T^-\widehat{\boldsymbol{E}}^{+} + \gamma_T^+\widehat{\boldsymbol{E}}^{-}\right]_\Gamma + \mathrm{Re}\left[\gamma_T^+\widehat{\boldsymbol{E}}^{-}, \gamma_T^-\widehat{\boldsymbol{H}}^{+} + \gamma_T^+\widehat{\boldsymbol{H}}^{-}\right]_\Gamma \\ &= \mathrm{Re}\left[\gamma_T^-\widehat{\boldsymbol{H}}^{+}, \gamma_T^-\widehat{\boldsymbol{E}}^{+}\right]_\Gamma - \mathrm{Re}\left[\gamma_T^+\widehat{\boldsymbol{H}}^{-}, \gamma_T^+\widehat{\boldsymbol{E}}^{-}\right]_\Gamma. \end{aligned}$$

As the direct consequence of (3.21), we observe that $(\widehat{\boldsymbol{E}}^{+}, \widehat{\boldsymbol{H}}^{+})|_{\Omega^-}$ and $(\widehat{\boldsymbol{E}}^{-}, \widehat{\boldsymbol{H}}^{-})|_{\Omega^+}$ vanish.

To obtain the bound (3.32), observe that we are now in the situation of Lemma 3.4, and the claim follows together with the bounds given in Proposition 3.9. Finally, the uniqueness of the boundary integral equation implies that there exists only a unique solution characterized by the representation formulas. We obtain the uniqueness of the fields $(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{H}}) \in H(\mathbf{curl}, \mathbb{R}^3 \setminus \Gamma)$ by observing that for $\mathrm{Re}\, s > 0$, any Maxwell solution in $H(\mathbf{curl}, \mathbb{R}^3 \setminus \Gamma)$ is characterized by the representation formula. □

Remark 3.11. In view of the L^2-bound of Lemma 3.4, we further obtain an improved L^2-bound for the solution of the time-harmonic scattering problem. Under the strong passivity condition (3.9) we have the bound

$$\left\| \begin{pmatrix} \widehat{\boldsymbol{E}} \\ \widehat{\boldsymbol{H}} \end{pmatrix} \right\|_{L^2(\Omega^\pm)^2} \leq C_{\Gamma,\sigma} \frac{|s|^2}{(\mathrm{Re}\, s)^{3/2}} \left\| \widehat{\boldsymbol{g}}^{\mathrm{inc}} \right\|_{\mathrm{X}_\Gamma{}^2} \qquad \text{for } \mathrm{Re}\, s \geq \sigma > 0.$$

3.5 The time-dependent scattering problem

3.5.1 The time-dependent boundary integral equation

Throughout this section we assume strong passivity condition (3.9). The time-dependent version of the boundary integral equation (3.29) is obtained by formally replacing the Laplace transform variable s by the time differentiation operator ∂_t: Given $\boldsymbol{g}^{\mathrm{inc}} : [0,T] \to \mathrm{X}_\Gamma{}^2$, find time-dependent boundary densities $(\boldsymbol{\phi}^+, \boldsymbol{\phi}^-) : [0,T] \to \mathrm{X}_\Gamma{}^2 \times \mathrm{X}_\Gamma{}^2$ (of temporal regularity to be specified later) such that for almost every $t \in [0,T]$ we have

$$\begin{pmatrix} \boldsymbol{C}_{\varepsilon^+,\mu^+}(\partial_t) & \boldsymbol{J} \\ -\boldsymbol{J} & \boldsymbol{C}_{\varepsilon^-,\mu^-}(\partial_t) \end{pmatrix} \begin{pmatrix} \boldsymbol{\phi}^+ \\ \boldsymbol{\phi}^- \end{pmatrix} = \begin{pmatrix} -\boldsymbol{g}^{\mathrm{inc}} \\ \boldsymbol{g}^{\mathrm{inc}} \end{pmatrix}. \tag{3.35}$$

We abbreviate this as

$$\boldsymbol{A}(\partial_t)\boldsymbol{\phi} = \boldsymbol{g} \quad \text{with} \quad \boldsymbol{\phi}(t) = \begin{pmatrix} \boldsymbol{\phi}^+(t) \\ \boldsymbol{\phi}^-(t) \end{pmatrix} \in {\mathrm{X}_\Gamma}^4, \quad \boldsymbol{g}(t) = \begin{pmatrix} -\boldsymbol{g}^{\mathrm{inc}}(t) \\ \boldsymbol{g}^{\mathrm{inc}}(t) \end{pmatrix} \in {\mathrm{X}_\Gamma}^4. \tag{3.36}$$

In view of the bound of Proposition 3.9 on the operator family $\boldsymbol{A}(s)^{-1}$ for $\operatorname{Re} s > 0$, the temporal convolution operator

$$\boldsymbol{A}^{-1}(\partial_t)\boldsymbol{g} = \mathcal{L}^{-1}\boldsymbol{A}^{-1} * \boldsymbol{g}$$

is well-defined, and by the composition rule we have $\boldsymbol{A}^{-1}(\partial_t)\boldsymbol{A}(\partial_t) = \mathbf{Id}$ and $\boldsymbol{A}(\partial_t)\boldsymbol{A}^{-1}(\partial_t) = \mathbf{Id}$. So we have the temporal convolution

$$\boldsymbol{\phi} = \boldsymbol{A}^{-1}(\partial_t)\boldsymbol{g}$$

as the unique solution of (3.36). More precisely, with the argument given above and the convolution bound of [95, Lemma 2.1], we obtain the following result. Here $H_0^r(0,T;{\mathrm{X}_\Gamma}^4)$ is the space of functions on the interval $(0,T)$ taking values in ${\mathrm{X}_\Gamma}^4$ that have an extension to the real line that is in the Sobolev space $H^r(\mathbb{R},{\mathrm{X}_\Gamma}^4)$.

Theorem 3.12 (Well-posedness of the time-dependent boundary integral equation)**.** *Let $r \geq 0$. For $\boldsymbol{g} \in H_0^{r+3}(0,T;{\mathrm{X}_\Gamma}^4)$, the boundary integral equation (3.36) has a unique solution $\boldsymbol{\phi} \in H_0^{r+1}(0,T;{\mathrm{X}_\Gamma}^4)$, and*

$$\|\boldsymbol{\phi}\|_{H_0^{r+1}(0,T;{\mathrm{X}_\Gamma}^4)} \leq C_T \ \|\boldsymbol{g}\|_{H_0^{r+3}(0,T;{\mathrm{X}_\Gamma}^4)}.$$

Here, C_T depends on T and on the boundary Γ via norms of tangential trace operators.

3.5.2 Well-posedness of the time-dependent scattering problem

With the time-dependent boundary densities $\boldsymbol{\phi} = (\boldsymbol{\phi}^+, \boldsymbol{\phi}^-)^T$ of Theorem 3.12, the scattered wave is obtained by the time-dependent representation formula, compactly denoted by the exterior and interior block operators $\boldsymbol{\mathcal{W}}^\pm(\partial_t)$ via

$$\begin{pmatrix} \boldsymbol{E}^\pm \\ \boldsymbol{H}^\pm \end{pmatrix} = \boldsymbol{\mathcal{W}}^\pm(\partial_t)\boldsymbol{\phi}^\pm = \begin{pmatrix} -\sqrt{\frac{\mu^\pm}{\varepsilon^\pm}}(\partial_t)\,\boldsymbol{\mathcal{S}}^\pm_{\varepsilon,\mu}(\partial_t)\boldsymbol{\varphi}^\pm + \boldsymbol{\mathcal{D}}^\pm_{\varepsilon,\mu}(\partial_t)\psi^\pm \\ -\boldsymbol{\mathcal{D}}^\pm_{\varepsilon,\mu}(\partial_t)\boldsymbol{\varphi}^\pm - \sqrt{\frac{\varepsilon^\pm}{\mu^\pm}}(\partial_t)\,\boldsymbol{\mathcal{S}}^\pm_{\varepsilon,\mu}(\partial_t)\,\psi^\pm \end{pmatrix}, \tag{3.37}$$

where we used (3.16) and (3.17).

We now give the well-posedness result for the time-dependent scattering problem, which follows from the time-harmonic well-posedness result Proposition 3.10.

Theorem 3.13 (Well-posedness of the time-dependent scattering problem)**.** *Consider the time-dependent scattering problem (3.7) equipped with (3.6) and $\boldsymbol{g}^{\mathrm{inc}} \in H_0^{r+3}(0,T;{\mathrm{X}_\Gamma}^2)$ for some arbitrary $r \geq 0$.*

(a) This problem has a unique solution

$$(\boldsymbol{E}^\pm, \boldsymbol{H}^\pm) \in H_0^r(0,T;H(\mathbf{curl},\Omega^\pm)^2) \cap H_0^{r+1}(0,T;(\boldsymbol{L}^2(\Omega^\pm))^2)$$

given by the representation formulas (3.37). The tangential traces are uniquely determined by the solution of the system of boundary integral equations of Theorem 3.12,

$$(\boldsymbol{\varphi}^\pm, \psi^\pm) = (\gamma_T\boldsymbol{H}^\pm, -\gamma_T\boldsymbol{E}^\pm) \in H_0^{r+1}(0,T;\mathrm{X}_\Gamma \times \mathrm{X}_\Gamma).$$

(b) The electromagnetic fields are bounded by

$$\|\boldsymbol{E}^{\pm}\|_{H_0^r(0,T;H(\mathbf{curl},\Omega^{\pm}))} + \|\boldsymbol{H}^{\pm}\|_{H_0^r(0,T;H(\mathbf{curl},\Omega^{\pm}))} \leq C_T \|\boldsymbol{g}^{\mathrm{inc}}\|_{H_0^{r+3}(0,T;\mathrm{X}_\Gamma{}^2)},$$

and the same bound is valid for the $H_0^{r+1}(0,T;(\boldsymbol{L}^2(\Omega^{\pm}))^2)$ *norms. Here,* C_T *depends polynomially on* T*, on the boundary* Γ *via norms of tangential trace operators, and on the bounds of the frequency dependent material parameters* ε, μ*.*

Proof. The proof is identical to [112, Thm. 4.2]. □

Remark 3.14 (On the assumption $r \geq 0$). In the Theorems 3.12–3.13, the assumption $r \geq 0$ ensures that the scattered wave is at least square integrable in time. By the general result [95, Lemma 2.1], our results generalize to incoming waves with less regularity, although the scattered wave is then (temporally) only bounded in a Sobolev space with a negative order.

3.6 Semi-discretization in time by Runge–Kutta convolution quadrature

3.6.1 Recap: Runge–Kutta convolution quadrature

To approximate the omnipresent temporal convolutions $K(\partial_t)g$, we will employ the convolution quadrature method based on Runge–Kutta time stepping schemes. In order to introduce the notation, we recall an m-stage implicit Runge–Kutta discretization of the initial value problem $y' = f(t,y)$, $y(0) = y_0$; see [63]. For some constant time step $\tau > 0$, the approximations y^n to $y(t_n)$ at time $t_n = n\tau$, and the internal stages Y^{ni} approximating $y(t_n + c_i\tau)$, are computed by solving the system

$$\begin{aligned} Y^{ni} &= y^n + \tau \sum_{j=1}^{m} a_{ij} f(t_n + c_j\tau, Y^{nj}), \qquad i = 1,\dots,m, \\ y^{n+1} &= y^n + \tau \sum_{j=1}^{m} b_j f(t_n + c_j\tau, Y^{nj}). \end{aligned}$$

The method is uniquely defined by the Butcher-tableau, which collects its coefficients

$$\mathscr{A} = (a_{ij})_{i,j=1}^m, \quad \boldsymbol{b} = (b_1,\dots,b_m)^T, \quad \text{and} \quad \boldsymbol{c} = (c_1,\dots,c_m)^T.$$

The stability function of the Runge–Kutta method is given by $R(z) = 1 + zb^T(\boldsymbol{I} - z\mathscr{A})^{-1}\mathbb{1}$, where $\mathbb{1} = (1,1,\dots,1)^T \in \mathbb{R}^m$. We always assume that $\mathscr{A}$ is invertible.

Runge–Kutta methods can be used to construct convolution quadrature methods. Such methods were first introduced in [99] in the context of parabolic problems and were studied for wave propagation problems in [15] and subsequently, e.g., in [10–12, 17]. Runge–Kutta convolution quadrature was studied for the numerical solution of some exterior Maxwell problems in [9, 40, 112] and of an eddy current problem with an impedance boundary condition in [75]. For wave problems, Runge–Kutta convolution quadrature methods such as those based on the Radau IIA methods, see [63, Section IV.5], often enjoy more favourable properties than their BDF-based counterparts, which are more dissipative and cannot exceed order 2 but are easier to understand and slightly easier to implement.

Let $\boldsymbol{K}(s) : \boldsymbol{X} \to \boldsymbol{Y}$, $\operatorname{Re} s \geq \sigma_0 > 0$, be an analytic family of linear operators between Banach spaces $\boldsymbol{X}$ and $\boldsymbol{Y}$, satisfying the bound, for some exponents $\kappa \in \mathbb{R}$ and $\nu \geq 0$,

$$\|\boldsymbol{K}(s)\|_{\boldsymbol{Y} \leftarrow \boldsymbol{X}} \leq M_\sigma \frac{|s|^\kappa}{(\operatorname{Re} s)^\nu}, \qquad \operatorname{Re} s \geq \sigma > \sigma_0. \tag{3.38}$$

This yields a convolution operator $\boldsymbol{K}(\partial_t) : H_0^{r+\kappa}(0,T;\boldsymbol{X}) \to \boldsymbol{H}_0^r(0,T;\boldsymbol{Y})$ for arbitrary real r. For functions $\boldsymbol{g} : [0,T] \to \boldsymbol{X}$ that are sufficiently regular (together with their extension by 0 to the negative real half-axis $t < 0$), we wish to approximate the convolution $(\boldsymbol{K}(\partial_t)\boldsymbol{g})(t)$ at discrete times $t_n = n\tau$ with a step size $\tau > 0$, using a discrete convolution.

To construct the convolution quadrature weights, we use the *Runge–Kutta differentiation symbol*

$$\Delta(\zeta) = \Big(\mathit{A} + \frac{\zeta}{1-\zeta} \mathbb{1} \boldsymbol{b}^T \Big)^{-1} \in \mathbb{C}^{m \times m}, \qquad \zeta \in \mathbb{C} \text{ with } |\zeta| < 1.$$

This is well-defined for $|\zeta| < 1$ if $R(\infty) = 1 - b^T \mathit{A}^{-1} \mathbb{1}$ satisfies $|R(\infty)| \leq 1$, as is seen from the Sherman–Woodbury formula. Moreover, for A-stable Runge–Kutta methods (e.g. the Radau IIA methods), the eigenvalues of the matrices $\Delta(\zeta)$ have positive real part for $|\zeta| < 1$ [15, Lemma 3].

To formulate the Runge–Kutta convolution quadrature for $\boldsymbol{K}(\partial_t)\boldsymbol{g}$, we replace the complex argument s in $\boldsymbol{K}(s)$ by the matrix $\Delta(\zeta)/\tau$ and expand

$$\boldsymbol{K}\Big(\frac{\Delta(\zeta)}{\tau}\Big) = \sum_{n=0}^{\infty} \boldsymbol{W}_n(\boldsymbol{K}) \zeta^n.$$

The operators $\boldsymbol{W}_n(\boldsymbol{K}) : \boldsymbol{X}^m \to \boldsymbol{Y}^m$ are used as the convolution quadrature "weights". For the discrete convolution of these operators with a sequence $\boldsymbol{g} = (\boldsymbol{g}^n)$ with $\boldsymbol{g}^n = (\boldsymbol{g}_i^n)_{i=1}^m \in \boldsymbol{X}^m$ we use the notation

$$\big(\boldsymbol{K}(\partial_t^\tau)\boldsymbol{g}\big)^n = \sum_{j=0}^{n} \boldsymbol{W}_{n-j}(\boldsymbol{K}) \boldsymbol{g}^j \in \boldsymbol{Y}^m. \tag{3.39}$$

Given a function $\boldsymbol{g} : [0,T] \to \boldsymbol{X}$, we use this notation for the vectors $\boldsymbol{g}^n = \big(\boldsymbol{g}(t_n + c_i\tau)\big)_{i=1}^m$ of values of $\boldsymbol{g}$. The i-th component of the vector $\big(\boldsymbol{K}(\partial_t^\tau)\boldsymbol{g}\big)^n$ is then an approximation to $\big(\boldsymbol{K}(\partial_t)\boldsymbol{g}\big)(t_n + c_i\tau)$; see [11, Theorem 4.2].

In particular, if $c_m = 1$, as is the case with Radau IIA methods, the continuous convolution at t_n is approximated by the m-th, i.e. last component of the m-vector (3.39) for $n-1$:

$$\big(\boldsymbol{K}(\partial_t)\boldsymbol{g}\big)(t_n) \approx \Big[\big(\boldsymbol{K}(\partial_t^\tau)\boldsymbol{g}\big)^{n-1}\Big]_m \in \boldsymbol{Y}.$$

This discretization (3.39) inherits the composition rule (3.12): For two analytic families of operators $\boldsymbol{K}(s)$ and $\boldsymbol{L}(s)$ mapping into compatible spaces, the convolution quadrature discretization satisfies

$$\boldsymbol{K}(\partial_t^\tau)\boldsymbol{L}(\partial_t^\tau)\boldsymbol{g} = (\boldsymbol{K}\boldsymbol{L})(\partial_t^\tau)\boldsymbol{g}; \tag{3.40}$$

see e.g. [95, Equation (3.5)].

The following error bound for Runge–Kutta convolution quadrature from [15], here directly stated for the Radau IIA methods [63, Section IV.5] and transferred to a Banach space setting, will be the basis for our error bounds of the time discretization.

Lemma 3.15 ([15, Theorem 3])**.** *Let $\boldsymbol{K}(s) : \boldsymbol{X} \to \boldsymbol{Y}$, $\operatorname{Re} s > \sigma_0 \geq 0$, be an analytic family of linear operators between Banach spaces $\boldsymbol{X}$ and $\boldsymbol{Y}$ satisfying the bound (3.38) with exponents κ and ν. Consider*

the Runge–Kutta convolution quadrature based on the Radau IIA method with m stages. Let $1 \leq q \leq m$ (the most interesting case is $q = m$) and $r > \max(2q + \kappa, 2q - 1, q + 1)$. Let $\boldsymbol{g} \in \boldsymbol{C}^r([0,T], \boldsymbol{X})$ satisfy $\boldsymbol{g}(0) = \boldsymbol{g}'(0) = \ldots = \boldsymbol{g}^{(r-1)}(0) = 0$. Then, the following error bound holds at $t_n = n\tau \in [0,T]$:

$$\begin{aligned}&\left\| \left[\left(\boldsymbol{K}(\partial_t^\tau)\boldsymbol{g} \right)^{n-1} \right]_m - (\boldsymbol{K}(\partial_t)\boldsymbol{g})(t_n) \right\|_{\boldsymbol{Y}} \\ &\qquad \leq C\, M_{1/T}\, \tau^{\min(2q-1, q+1-\kappa+\nu)} \left(\|\boldsymbol{g}^{(r)}(0)\|_{\boldsymbol{X}} + \int_0^t \|\boldsymbol{g}^{(r+1)}(\theta)\|_{\boldsymbol{X}} \,\mathrm{d}\theta \right).\end{aligned}$$

The constant C is independent of τ and $\boldsymbol{g}$ and M_σ of (3.38), but depends on the exponents κ and ν in (3.38) and on the final time T.

3.6.2 Convolution quadrature for the scattering problem

Throughout the following sections, we assume strong passivity (3.9) for the frequency dependent parameters $\varepsilon(s), \mu(s)$. Applying a Runge–Kutta based convolution quadrature discretization to the temporal convolution equation (3.36) reads

$$\boldsymbol{A}(\partial_t^\tau)\boldsymbol{\phi}_\tau = \boldsymbol{g}, \qquad \text{or equivalently,} \qquad \boldsymbol{\phi}_\tau = \boldsymbol{A}^{-1}(\partial_t^\tau)\, \boldsymbol{g},$$

where $\boldsymbol{\phi}$ and $\boldsymbol{g}$ are defined in (3.36), and the equivalence of the two formulations is a consequence of the discrete composition rule (3.40).

This formulation, which is equivalent to discretizing the boundary integral equation (3.36) with the convolution quadrature method and inverting the quadrature weights, interprets the solution of the discretized boundary integral equation as a forward convolution quadrature. The error of this formulation is then bounded by the error estimate of Lemma 3.15, through the bound of $\boldsymbol{A}^{-1}(s)$ given in Proposition 3.9. This argument for the stability of the formulation and the resulting path to error estimates originates from [95], for a time-dependent boundary integral equation derived in the context of an acoustic problem.

The time discretizations of the electromagnetic fields are then obtained by applying the convolution quadrature to the representation formulas (3.37) with $\boldsymbol{\phi}_\tau^\pm = (\boldsymbol{\varphi}_\tau^\pm, \psi_\tau^\pm)$:

$$\begin{pmatrix} \boldsymbol{E}_\tau^\pm \\ \boldsymbol{H}_\tau^\pm \end{pmatrix} = \boldsymbol{\mathcal{W}}^\pm(\partial_t^\tau)\boldsymbol{\phi}_\tau^\pm = \begin{pmatrix} -\sqrt{\frac{\mu^\pm}{\varepsilon^\pm}}(\partial_t^\tau)\, \boldsymbol{\mathcal{S}}_{\varepsilon,\mu}^\pm(\partial_t^\tau)\boldsymbol{\varphi}_\tau^\pm + \boldsymbol{\mathcal{D}}_{\varepsilon,\mu}^\pm(\partial_t^\tau)\psi_\tau^\pm \\ -\boldsymbol{\mathcal{D}}_{\varepsilon,\mu}^\pm(\partial_t^\tau)\boldsymbol{\varphi}_\tau^\pm - \sqrt{\frac{\varepsilon^\pm}{\mu^\pm}}(\partial_t^\tau)\, \boldsymbol{\mathcal{S}}_{\varepsilon,\mu}^\pm(\partial_t^\tau)\, \psi_\tau^\pm \end{pmatrix}.$$

By the discrete composition rule (3.40), this is the convolution quadrature discretization of the composed operator

$$\begin{pmatrix} \boldsymbol{E}_\tau^\pm \\ \boldsymbol{H}_\tau^\pm \end{pmatrix} = \boldsymbol{\mathcal{U}}^\pm(\partial_t^\tau)\boldsymbol{g}^{\mathrm{inc}} \qquad \text{of} \qquad \begin{pmatrix} \boldsymbol{E}^\pm \\ \boldsymbol{H}^\pm \end{pmatrix} = \boldsymbol{\mathcal{U}}^\pm(\partial_t)\boldsymbol{g}^{\mathrm{inc}}, \tag{3.41}$$

where we have by Theorem 3.13 that is given by

$$\boldsymbol{\mathcal{U}}^\pm(s) = \boldsymbol{\mathcal{W}}^\pm(s)\boldsymbol{\mathcal{P}}^\pm \boldsymbol{A}^{-1}(s)\boldsymbol{\mathcal{N}}, \tag{3.42}$$

with the auxiliary maps $\boldsymbol{\mathcal{P}}^\pm \colon \mathrm{X}_\Gamma{}^4 \to \mathrm{X}_\Gamma{}^2$ projecting on the exterior and interior boundary densities respectively and $\boldsymbol{\mathcal{N}} \colon \mathrm{X}_\Gamma{}^2 \to \mathrm{X}_\Gamma{}^4$ expanding the terms of the incident wave via

$$\boldsymbol{\mathcal{P}}^+ = \begin{pmatrix} \mathbf{Id} & 0 \end{pmatrix}, \quad \boldsymbol{\mathcal{P}}^- = \begin{pmatrix} 0 & \mathbf{Id} \end{pmatrix} \quad \text{and} \quad \boldsymbol{\mathcal{N}} = \begin{pmatrix} -\mathbf{Id} & \mathbf{Id} \end{pmatrix}^\top.$$

Under the stronger passivity condition, we then have by Proposition 3.10 and Remark 3.11 the bound

$$\|\boldsymbol{\mathcal{U}}^{\pm}(s)\|_{H(\mathbf{curl},\Omega^{\pm})^2\leftarrow \mathrm{X}_\Gamma{}^2} \leq C_\sigma \frac{|s|^3}{(\operatorname{Re} s)^{3/2}}, \quad \text{for } \operatorname{Re} s \geq \sigma > 0. \tag{3.43}$$

Moreover, away from the boundary on $\Omega_d^{\pm} = \{x \in \Omega^{\pm} : \operatorname{dist}(x,\Gamma) > d\}$ with $d > 0$, bounds that decay exponentially with the real part of s hold. The following lemma is a direct consequence of [112, Lemma 3.8] and of Lemma 3.2 to obtain the following parameter-dependent bound.

Lemma 3.16. *Under the strong passivity condition (3.9), we have the following bounds at $\boldsymbol{x} \in \mathbb{R}^3 \setminus \Gamma$ with $d = \operatorname{dist}(x,\Gamma) > 0$ and for $\operatorname{Re} s \geq \sigma > 0$*

$$\begin{aligned} \big|\big(\boldsymbol{\mathcal{S}}_{\varepsilon,\mu}(s)\varphi\big)(x)\big| &\leq C_\sigma\, |s|^2\, \mathrm{e}^{-dc\operatorname{Re} s}\, \|\varphi\|_{\mathrm{X}_\Gamma}\,, \\ \big|\big(\boldsymbol{\mathcal{D}}_{\varepsilon,\mu}(s)\varphi\big)(x)\big| &\leq C_\sigma\ |s|^2\, \mathrm{e}^{-dc\operatorname{Re} s}\, \|\varphi\|_{\mathrm{X}_\Gamma}\,. \end{aligned}$$

for all $\varphi \in \mathrm{X}_\Gamma$.

Combining Lemma 3.16 and Proposition 3.9 yields, under the assumption of strong passivity (3.9) and using (3.20),

$$\|\boldsymbol{\mathcal{U}}^{\pm}(s)\|_{(\boldsymbol{C}^1(\overline{\Omega}_d^{\pm})^3)^2\leftarrow \mathrm{X}_\Gamma{}^2} \leq C_\sigma \frac{|s|^{1/2}}{(\operatorname{Re} s)^{1/2}} \frac{|s|^4}{\operatorname{Re} s} e^{-dc\operatorname{Re} s}\ \big\|\widehat{\boldsymbol{g}}^{\mathrm{inc}}\big\|_{\mathrm{X}_\Gamma{}^2}\,, \tag{3.44}$$

for $\operatorname{Re} s \geq \sigma > 0$. The $\boldsymbol{C}^1(\overline{\Omega}_d^{\pm})$-norm denotes the maximum norm on continuously differentiable functions and their derivatives on the closure of the domains $\Omega_d^{\pm}$ respectively.

For the sake of brevity, we omit a formulation of error bounds for the temporal semi-discretization and continue with a full discretization for the boundary integral equation.

3.7 Full discretization

Finally, we combine a convolution quadrature time discretization of (3.36) with a spatial Galerkin approximation of the boundary operators, based on a boundary element space $\boldsymbol{X}_h \subset \mathrm{X}_\Gamma$, which corresponds to a family of triangulations with decreasing mesh width $h \to 0$. Throughout this paper, we use Raviart–Thomas boundary elements of order $k \geq 0$, which are defined on the unit triangle $\widehat{K}$ by

$$\mathrm{RT}_k(\widehat{K}) = \Big\{ x \mapsto \boldsymbol{p}_1(x) + p_2(x)x \,:\, \boldsymbol{p}_1 \in P_k(\widehat{K})^2,\ p_2 \in P_k(\widehat{K}) \Big\},$$

where $P_k(\widehat{K})$ contains all polynomials of degree k on $\widehat{K}$. The definition is then extended to arbitrary triangles in the standard way via pull-back to the reference element. Details are found in the original paper [119].

The following approximation result holds with respect to the X_Γ-norm; see also the original references [26, Section III.3.3] and [28]. Here we use the same notation $H_\times^p(\Gamma) = \gamma_T H^{p+1/2}(\Omega)$ as in [29].

Lemma 3.17 ([29, Theorem 14])**.** *Let $\boldsymbol{X}_h$ be the k-th order Raviart–Thomas boundary element space on Γ. There exists a constant C, such that the best-approximation error of any $\boldsymbol{\xi} \in \mathrm{X}_\Gamma \cap H_\times^{k+1}(\Gamma)$ is bounded by*

$$\inf_{\boldsymbol{\xi}_h \in \boldsymbol{X}_h} \|\boldsymbol{\xi}_h - \boldsymbol{\xi}\|_{\mathrm{X}_\Gamma} \leq C h^{k+3/2} \|\boldsymbol{\xi}\|_{H_\times^{k+1}(\Gamma)}.$$

The full discretization of boundary integral equation (3.36) on $\boldsymbol{X}_h^4$ then reads

$$[\boldsymbol{\xi}_h\,,\,\boldsymbol{A}(\partial_t^\tau)\boldsymbol{\phi}_h^\tau]_\Gamma = [\,\boldsymbol{\xi}_h\,,\,\boldsymbol{g}_{\mathrm{inc}}]_\Gamma \qquad \forall\,\boldsymbol{\xi}_h \in (\boldsymbol{X}_h^4)^m. \tag{3.45}$$

This formulation determines the approximate boundary densities, by

$$(\boldsymbol{\phi}_h^\tau)^n = \Big((\varphi_{\tau,h}^+)^n, (\psi_{\tau,h}^+)^n, (\varphi_{\tau,h}^-)^n, (\psi_{\tau,h}^+)^n\Big)^\top \in \boldsymbol{X}_h^4,$$

where $\boldsymbol{\varphi}_{\tau,h}^\pm = \big((\boldsymbol{\varphi}_{\tau,h}^\pm)^n\big)$ with $(\boldsymbol{\varphi}_{\tau,h}^\pm)^n = \big((\boldsymbol{\varphi}_{\tau,h}^\pm)_i^n\big)_{i=1}^m \in \boldsymbol{X}_h^m$. The electric densities $\psi_{\tau,h}^\pm$ are defined in the same way. The approximations to the electromagnetic fields are obtained via the time-discrete representation formulas on the interior domain Ω^- and the exterior domain Ω^+:

$$\boldsymbol{E}_{\tau,h}^\pm = -\sqrt{\frac{\mu}{\varepsilon}}(\partial_t^\tau)\,\boldsymbol{\mathcal{S}}_{\varepsilon,\mu}(\partial_t^\tau)\boldsymbol{\varphi}_{\tau,h}^\pm + \boldsymbol{\mathcal{D}}_{\varepsilon,\mu}(\partial_t^\tau)\psi_{\tau,h}^\pm, \tag{3.46}$$

$$\boldsymbol{H}_{\tau,h}^\pm = -\boldsymbol{\mathcal{D}}_{\varepsilon,\mu}(\partial_t^\tau)\boldsymbol{\varphi}_{\tau,h}^\pm - \sqrt{\frac{\varepsilon}{\mu}}(\partial_t^\tau)\,\boldsymbol{\mathcal{S}}_{\varepsilon,\mu}(\partial_t^\tau)\psi_{\tau,h}^\pm. \tag{3.47}$$

These fully discrete approximations satisfy the following error bounds, obtained under regularity assumptions that are presumably stronger than necessary.

Theorem 3.18 (Error bound of the full discretization)**.** *Consider the setting and assumptions of Theorem 3.13 and further let $\varepsilon^\pm$ and $\mu^\pm$ satisfy the strong passivity (3.9).*

Consider the fully discrete scheme (3.45) and the temporally discrete representation formulas (3.46)–(3.47), where the $m-$stage Radau IIA convolution quadrature discretization and k-th order Raviart–Thomas boundary element discretization have been employed as described in the previous sections.
For $r > 2m+4$ we assume the incoming waves to satisfy $\boldsymbol{g}^{\mathrm{inc}} \in \boldsymbol{C}^r([0,T], \mathrm{X}_\Gamma{}^4)$. Moreover, we assume $\boldsymbol{g}^{\mathrm{inc}}$ to vanish at $t=0$ together with its first $r-1$ time derivatives. Furthermore, it is assumed that the solution $\boldsymbol{\phi}$ of the boundary integral equation (3.36) is at least in $\boldsymbol{C}^{10}([0,T], H_\times^{k+1}(\Gamma)^2)$, vanishing at $t=0$ together with its time derivatives.
Then, the approximations to the electromagnetic fields at time t_n, both in the interior and the exterior domain,

$$\Big(\boldsymbol{E}_{\tau,h}^\pm\Big)^n = \big[(\boldsymbol{E}_{\tau,h}^\pm)^{n-1}\big]_m \quad \text{and} \quad \Big(\boldsymbol{H}_{\tau,h}^\pm\Big)^n = \big[(\boldsymbol{H}_{\tau,h}^\pm)^{n-1}\big]_m,$$

satisfy the following error bound of order $m-1/2$ in time and order $k+3/2$ in space at $t_n = n\tau \in [0,T]$:

$$\Big\|\Big(\boldsymbol{E}_{\tau,h}^\pm\Big)^n - \boldsymbol{E}(t_n)\Big\|_{H(\mathbf{curl},\Omega^\pm)} + \Big\|\Big(\boldsymbol{H}_{\tau,h}^\pm\Big)^n - \boldsymbol{H}(t_n)\Big\|_{H(\mathbf{curl},\Omega^\pm)} \le C\big(\tau^{m-1/2} + h^{k+3/2}\big).$$

For $r > 2m+4$, we obtain the full order $2m-1$ in time away from the interface Γ, on the domains $\Omega_d^\pm = \{x \in \Omega : \operatorname{dist}(x,\Gamma) > d\}$ with $d > 0$, which reads

$$\Big\|\Big(\boldsymbol{E}_{\tau,h}^\pm\Big)^n - \boldsymbol{E}(t_n)\Big\|_{\boldsymbol{C}^1(\overline{\Omega}_d^\pm)^3} + \Big\|\Big(\boldsymbol{H}_{\tau,h}^\pm\Big)^n - \boldsymbol{H}(t_n)\Big\|_{\boldsymbol{C}^1(\overline{\Omega}_d^\pm)^3} \le C_d\big(\tau^{2m-1} + h^{k+3/2}\big).$$

The constants C and C_d are independent of n, τ and h, but depend on the final time T and on the regularity of $\boldsymbol{g}^{\mathrm{inc}}$ and $(\boldsymbol{\varphi},\psi)$ as stated. C_d additionally depends on the distance d.

Proof. The proof is, due to the similarities of the time-harmonic bounds, essentially identical to the proof of [112, Theorem 6.1]. We repeat the arguments given there and apply them to the present setting, to keep the paper self-contained. We structure the proof into three parts (a)–(c).

(a) *(Discretized time-harmonic boundary integral equation).* We start with the time-harmonic boundary integral equation (3.30), for $\operatorname{Re} s > 0$. We denote by $\boldsymbol{L}_h(s) : {\mathrm{X}_\Gamma}^4 \to \boldsymbol{X}_h^4$ the solution operator $\widehat{\boldsymbol{g}} \mapsto \widehat{\boldsymbol{\phi}_h}$ of the Galerkin approximation in $\boldsymbol{X}_h^4$,

$$\left[\boldsymbol{\xi}_h, \boldsymbol{A}(s)\widehat{\boldsymbol{\phi}}_h\right]_\Gamma = [\boldsymbol{\xi}_h, \widehat{\boldsymbol{g}}]_\Gamma \qquad \forall\, \boldsymbol{\xi}_h \in \boldsymbol{X}_h^4,$$

which by the bound of $\boldsymbol{A}(s)$ in Lemma 3.7, the coercivity estimate of Lemma 3.8 and the Lax–Milgram lemma yields, for $\operatorname{Re} s \geq \sigma > 0$, the bound

$$\|\boldsymbol{L}_h(s)\|_{\boldsymbol{X}_h^4 \leftarrow {\mathrm{X}_\Gamma}^4} \leq C_\sigma \frac{|s|^2}{\operatorname{Re} s}, \tag{3.48}$$

where C_σ depends on the surface Γ and σ. The associated Ritz projection $\boldsymbol{R}_h(s) : {\mathrm{X}_\Gamma}^4 \to \boldsymbol{X}_h^4$ maps $(\widehat{\boldsymbol{\phi}}) \in {\mathrm{X}_\Gamma}^4$ to $\widehat{\boldsymbol{\phi}}_h \in \boldsymbol{X}_h^4$, determined by

$$\left[\boldsymbol{\xi}_h, \boldsymbol{A}(s)\widehat{\boldsymbol{\phi}}_h\right]_\Gamma = \left[\boldsymbol{\xi}_h, \boldsymbol{A}(s)\widehat{\boldsymbol{\phi}}\right]_\Gamma \qquad \forall\, \boldsymbol{\xi}_h \in \boldsymbol{X}_h^4.$$

Again by Lemmas 3.7 and 3.8 and the Lax–Milgram lemma, this problem has a unique solution $(\widehat{\boldsymbol{\varphi}}_h, \widehat{\boldsymbol{\psi}}_h) \in \boldsymbol{X}_h^4$, and by Céa's lemma, where the right-hand side is further bounded by Lemma 3.17. With the stronger passivity, we arrive at the bound

$$\left\|\widehat{\boldsymbol{\phi}}_h - \widehat{\boldsymbol{\phi}}\right\|_{{\mathrm{X}_\Gamma}^4} \leq \frac{C_\sigma}{c_\sigma} \left(\frac{|s|^2}{\operatorname{Re} s}\right)^2 \inf_{\boldsymbol{\xi}_h \in \boldsymbol{X}_h^4} \left\|\boldsymbol{\xi}_h - \widehat{\boldsymbol{\phi}}\right\|_{{\mathrm{X}_\Gamma}^4},$$

for all $\operatorname{Re} s \geq \sigma > 0$.

In combination with the approximation result of Lemma 3.17, we can thus bound the associated error operator $\boldsymbol{\mathcal{E}}_h(s) = \boldsymbol{R}_h(s) - \mathbf{Id}$ in the operator norm from $H_\times^{k+1}(\Gamma)^4$ to ${\mathrm{X}_\Gamma}^4$ with the bound, for $\operatorname{Re} s \geq \sigma > 0$,

$$\|\boldsymbol{\mathcal{E}}_h(s)\|_{\mathrm{V}_\Gamma \times \mathrm{X}_\Gamma \leftarrow H_\times^{k+1}(\Gamma)^2} \leq \widetilde{C}_\sigma \frac{|s|^4}{(\operatorname{Re} s)^2}\, h^{k+3/2}. \tag{3.49}$$

(b) *(Error of the spatial semi-discretization).* We continue with the spatial semi-discretization of the time-dependent boundary integral equation (3.36), which reads

$$[\boldsymbol{\xi}_h, \boldsymbol{A}(\partial_t)\boldsymbol{\phi}] = [\boldsymbol{\xi}_h, \boldsymbol{g}]_\Gamma \qquad \forall\, \boldsymbol{\xi}_h \in \boldsymbol{X}_h^4.$$

This formulation has the unique solution

$$\boldsymbol{\phi}_h = \boldsymbol{L}_h(\partial_t)\boldsymbol{g} = \boldsymbol{R}_h(\partial_t)\boldsymbol{\phi},$$

where $\boldsymbol{\phi} = \boldsymbol{A}^{-1}(\partial_t)\boldsymbol{g}$ is the solution of (3.36). With the exterior and interior potential operators collected in the block operators $\boldsymbol{\mathcal{W}}^\pm(s)$ and the auxiliary operators $\boldsymbol{\mathcal{P}}^\pm$ and $\boldsymbol{\mathcal{N}}$ defined in (3.42) we set

$$\boldsymbol{\mathcal{U}}_h^\pm(s) = \boldsymbol{\mathcal{W}}^\pm(s)\boldsymbol{\mathcal{P}}^\pm \boldsymbol{L}_h(s)\boldsymbol{\mathcal{N}} \colon {\mathrm{X}_\Gamma}^2 \to H(\mathbf{curl}, \Omega^\pm)^2. \tag{3.50}$$

With the established bounds from Lemma 3.3 and (3.48), this operator family is bounded by

$$\|\boldsymbol{\mathcal{U}}_h^\pm(s)\|_{H(\mathbf{curl},\Omega^\pm)^2 \leftarrow {\mathrm{X}_\Gamma}^2} \leq \bar{C}_\sigma \frac{|s|^4}{(\operatorname{Re} s)^2}.$$

The spatial semi-discretization of the scattering problem is then the forward convolution of $\boldsymbol{\mathcal{U}}_h^\pm(\partial_t)$ with the incident wave, which reads

$$\begin{pmatrix} \boldsymbol{E}_h^\pm \\ \boldsymbol{H}_h^\pm \end{pmatrix} = \boldsymbol{\mathcal{U}}_h^\pm(\partial_t)\boldsymbol{g}^{\mathrm{inc}}.$$

In view of (3.41), its error is

$$\begin{aligned}\begin{pmatrix}\boldsymbol{E}_h^\pm\\ \boldsymbol{H}_h^\pm\end{pmatrix}-\begin{pmatrix}\boldsymbol{E}^\pm\\ \boldsymbol{H}^\pm\end{pmatrix}&=\boldsymbol{\mathcal{U}}_h^\pm(\partial_t)\boldsymbol{g}^{\mathrm{inc}}-\boldsymbol{\mathcal{U}}^\pm(\partial_t)\boldsymbol{g}^{\mathrm{inc}}=\boldsymbol{\mathcal{W}}^\pm(\partial_t)\boldsymbol{\phi}_h^\pm-\boldsymbol{\mathcal{W}}^\pm(\partial_t)\boldsymbol{\phi}^\pm\\ &=\boldsymbol{\mathcal{W}}^\pm(\partial_t)(\boldsymbol{R}_h-\mathbf{Id})\boldsymbol{\phi}^\pm=\boldsymbol{\mathcal{W}}^\pm(\partial_t)\,\boldsymbol{\mathcal{E}}_h(\partial_t)\boldsymbol{\phi}^\pm.\end{aligned}$$

Using the bound of Lemma 3.3 for the potential operator $\boldsymbol{\mathcal{W}}^\pm(s)$, the bound (3.49) for the error operator $\boldsymbol{\mathcal{E}}_h(s)$, and the temporal Sobolev bound stated in [95, Lemma 2.1] (with $\kappa=6$) for their composition, and finally the Sobolev embedding $H^1(0,T;H)\subset C([0,T],H)$ for any Hilbert space H, we obtain for the error of the spatial semi-discretization

$$\begin{aligned}&\max_{0\le t\le T}\left\|\begin{pmatrix}\boldsymbol{E}_h^\pm(t)\\ \boldsymbol{H}_h^\pm(t)\end{pmatrix}-\begin{pmatrix}\boldsymbol{E}^\pm(t)\\ \boldsymbol{H}^\pm(t)\end{pmatrix}\right\|_{H(\mathbf{curl},\Omega^\pm)^2}\\ &\le C\left\|\begin{pmatrix}\boldsymbol{E}_h^\pm\\ \boldsymbol{H}_h^\pm\end{pmatrix}-\begin{pmatrix}\boldsymbol{E}^\pm\\ \boldsymbol{H}^\pm\end{pmatrix}\right\|_{H_0^1(0,T;H(\mathbf{curl},\Omega^\pm)^2)}\le C_T\,h^{k+3/2}\left\|\boldsymbol{\phi}^\pm\right\|_{H_0^7(0,T;H_\times^{k+1}(\Gamma)^2)}.\end{aligned}\tag{3.51}$$

Using the same argument with the pointwise bounds away from the boundary given by Lemma 3.16, we further obtain

$$\max_{0\le t\le T}\left\|\begin{pmatrix}\boldsymbol{E}_h^\pm(t)\\ \boldsymbol{H}_h^\pm(t)\end{pmatrix}-\begin{pmatrix}\boldsymbol{E}^\pm(t)\\ \boldsymbol{H}^\pm(t)\end{pmatrix}\right\|_{\boldsymbol{C}^1(\overline{\Omega}_d^\pm)^2}\le C_T\,h^{k+3/2}\left\|\boldsymbol{\phi}^\pm\right\|_{H_0^9(0,T;H_\times^{k+1}(\Gamma)^4)}.$$

(c) *(Error of the full discretization).* The total error is (omitting here the omnipresent superscript n)

$$\begin{pmatrix}\boldsymbol{E}_{\tau,h}^\pm\\ \boldsymbol{H}_{\tau,h}^\pm\end{pmatrix}-\begin{pmatrix}\boldsymbol{E}_\tau^\pm\\ \boldsymbol{H}_\tau^\pm\end{pmatrix}\quad+\quad\begin{pmatrix}\boldsymbol{E}_\tau^\pm\\ \boldsymbol{H}_\tau^\pm\end{pmatrix}-\begin{pmatrix}\boldsymbol{E}^\pm\\ \boldsymbol{H}^\pm\end{pmatrix}.\tag{3.52}$$

The second difference is the error of the temporal semi-discretization, which is bounded by applying Lemma 3.39 with the time-harmonic bounds on $\boldsymbol{\mathcal{U}}^\pm(s)$ due to

$$\begin{pmatrix}\boldsymbol{E}_\tau^\pm\\ \boldsymbol{H}_\tau^\pm\end{pmatrix}-\begin{pmatrix}\boldsymbol{E}^\pm\\ \boldsymbol{H}^\pm\end{pmatrix}=\left(\boldsymbol{\mathcal{U}}^\pm(\partial_t^\tau)-\boldsymbol{\mathcal{U}}^\pm(\partial_t)\right)\boldsymbol{g}^{\mathrm{inc}}.$$

With the time-harmonic bound (3.43), we obtain an estimate of the order $O(\tau^{m-1/2})$ in the $H(\mathbf{curl},\Omega^\pm)$-norm, whereas applying the time-harmonic (3.44) yields an error estimate of the order $O(\tau^{2m-1})$ in the $\boldsymbol{C}^1(\overline{\Omega}_d^\pm)$-norm.

The first difference of the total error (3.52) is rewritten as

$$\begin{aligned}\boldsymbol{\mathcal{W}}^\pm(\partial_t^\tau)\boldsymbol{\mathcal{E}}_h(\partial_t^\tau)\boldsymbol{\phi}^\pm&=\left(\boldsymbol{\mathcal{W}}^\pm(\partial_t^\tau)\boldsymbol{\mathcal{E}}_h(\partial_t^\tau)\boldsymbol{\phi}^\pm-\boldsymbol{\mathcal{W}}^\pm(\partial_t)\boldsymbol{\mathcal{E}}_h(\partial_t)\boldsymbol{\phi}^\pm\right)\\ &+\ \boldsymbol{\mathcal{W}}^\pm(\partial_t)\boldsymbol{\mathcal{E}}_h(\partial_t)\boldsymbol{\phi}^\pm.\end{aligned}$$

The final error term is the spatial semi-discretization studied in part (b), which is therefore bounded by (3.51). To bound the remaining difference, which is a convolution quadrature error, we employ Lemma 3.15. This gives an $O(h^{k+3/2})$ error in the $H(\mathbf{curl},\Omega^\pm)^2$ norm, using that by Lemma 3.3 and (3.49) we have here $M_\sigma\le C_\sigma h^{k+3/2}$, $\kappa=6$, $\nu=3$ in (3.38) with $\boldsymbol{\mathcal{W}}(s)\boldsymbol{\mathcal{E}}_h(s)$ in the role of $\boldsymbol{K}(s)$, and choosing $q=2$ and $r=10>2q-1+\kappa$. Note that here $\min(2q-1,q+1-\kappa+\nu)=q-2=0$. Altogether, this yields the stated $O(\tau^{m-1/2}+h^{k+3/2})$ error bound in the $H(\mathbf{curl},\Omega^\pm)^2$ norm.

The full-order error bound away from the boundary can be shown without requiring this additional assumption on r. To show this bound, we rewrite the error as

$$\begin{pmatrix} \begin{pmatrix} \boldsymbol{E}^{\pm}_{\tau,h} \end{pmatrix}^n \\ \begin{pmatrix} \boldsymbol{H}^{\pm}_{\tau,h} \end{pmatrix}^n \end{pmatrix} - \begin{pmatrix} \boldsymbol{E}^{\pm}_{h}(t_n) \\ \boldsymbol{E}^{\pm}_{h}(t_n) \end{pmatrix} \quad + \quad \begin{pmatrix} \boldsymbol{E}^{\pm}_{h}(t_n) \\ \boldsymbol{E}^{\pm}_{h}(t_n) \end{pmatrix} - \begin{pmatrix} \boldsymbol{E}^{\pm}(t_n) \\ \boldsymbol{H}^{\pm}(t_n) \end{pmatrix}.$$

The second difference is the error of the spatial semi-discretization studied in part (b). The first difference is a convolution quadrature error for the transfer operator $\boldsymbol{\mathcal{U}}^{\pm}_h(s)$ of (3.50):

$$\begin{pmatrix} \begin{pmatrix} \boldsymbol{E}^{\pm}_{\tau,h} \end{pmatrix}^n \\ \begin{pmatrix} \boldsymbol{H}^{\pm}_{\tau,h} \end{pmatrix}^n \end{pmatrix} - \begin{pmatrix} \boldsymbol{E}^{\pm}_{h}(t_n) \\ \boldsymbol{H}^{\pm}_{h}(t_n) \end{pmatrix} = \left[\left(\boldsymbol{\mathcal{U}}^{\pm}_h(\partial_t^\tau) \boldsymbol{g}^{\mathrm{inc}} \right)^{n-1} \right]_m - \boldsymbol{\mathcal{U}}^{\pm}_h(\partial_t) \boldsymbol{g}^{\mathrm{inc}}(t_n).$$

Using this argument to bound the error in the $H(\mathbf{curl}, \Omega^{\pm})$ norm by Lemma 3.15 would reduce the predicted error rate to $O(\tau^{m-1})$, hence the different argument structure before.

The exponential decay in the bound (3.44) exceeds any polynomial decay, which gives with (3.48) a constant $C_{\sigma,d}$, depending only on σ and d, such that

$$\|\boldsymbol{\mathcal{U}}^{\pm}_h(s)\|_{(\boldsymbol{C}^1(\overline{\Omega}^{\pm}_d)^3)^2 \leftarrow \mathrm{X}_\Gamma{}^2} \leq C_{\sigma,d} \frac{|s|^{\frac{9}{2}}}{(\operatorname{Re} s)^{\frac{3}{2}+m+1}} \left\| \widehat{\boldsymbol{g}}^{\mathrm{inc}} \right\|_{\mathrm{X}_\Gamma{}^2}, \tag{3.53}$$

for $\operatorname{Re} s \geq \sigma > 0$, by using $e^{-x} \leq C x^{-m-1}$ for $x \geq \sigma$. We then obtain the stated full convergence rates in the $H(\mathbf{curl}, \Omega^{\pm}_d)$ norm and the $\boldsymbol{C}^1(\overline{\Omega}^{\pm}_d)$ norm by Lemma 3.15, with $r > 2m + 7/2$ and κ, ν chosen accordingly to the bound above. □

Remark 3.19 (On regularity assumptions). Theorem 3.18 imposes rather strict regularity assumptions on the exact solution and predicts, under these assumptions, optimal temporal convergence rates. Under lower regularity assumptions on the exact solution, we do not expect our error analysis to be optimal. Possible extensions of our theory could be based on semigroup theory (see [12]) or on energy estimates (see [109, Theorem 2]). None of these approaches, however, can be used to derive pointwise error estimates of full classical order, as they appear in Theorem 3.18.

3.8 Numerical experiments

We complement the theory of the previous sections by the following experiments. The boundary element approximations of the boundary and potential operators of the Maxwell problem were realized by the library Bempp, which is described in [126]. The codes used to generate the simulation data and the figures are available via github.[1]

All experiments have been conducted with the following setting. One or several scatterers are illuminated by an incoming plane wave of the form

$$\boldsymbol{E}_{\mathrm{inc}}(\boldsymbol{x}, t) = \boldsymbol{p} e^{-c\|\boldsymbol{d}\cdot\boldsymbol{x}+t-t_0\|^2}, \tag{3.54}$$

The polarization vector is set to $\boldsymbol{p} = \frac{1}{\sqrt{2}}(-1, 0, -1)^T$, the direction to $\boldsymbol{d} = \frac{1}{\sqrt{2}}((-1, 0, 1)^T$ and the temporal shift to $t_0 = 4$. The incoming wave is smooth, however its tangential trace γ_T at the time $t = 0$ does

[1] https://github.com/joergnick/cqExperiments, last accessed on 25/10/2023.

not vanish. Consequently, the regularity assumptions of the error analysis (see e.g. Theorem 3.18) are technically not fulfilled, although the margin of error falls well beyond the machine precision and has no apparent effect on our experiments. From the point of view of this paper, we can interpret these defects as roundoff errors and refer the reader to [14, Section 3.4], for a discussion on their effects. We observe the interaction of the wave with different scatterers until the final time $T = 8$. The physical constants in the exterior domain Ω^+ are set to one, i.e. $\varepsilon^+ = \mu^+ = 1$. Inside the obstacle, we enforce a fractional material law, which reads

$$\varepsilon^-(s) = \frac{1}{2} + \frac{1}{1 + s^{1/2}}, \quad \mu^-(s) = \frac{1}{2}. \tag{3.55}$$

The corresponding time-varying material law includes fractional time derivatives and is therefore nonlocal in time. Moreover, since $\varepsilon^-(s)$ is not a rational function, techniques based on memory variables are not available.

3.8.1 Scattering from a sphere: Convergence plots

To investigate empirical convergence rates, we consider the following simple setting. The exterior of a unit sphere centered at the origin is initially at rest and excited by the plane wave (3.54) with $c = 10$. A sequence of grids, with the mesh widths $h_j = 2^{-j/2}$ for $j = 0, ..., 5$ is used with 0-th order Raviart–Thomas elements as the space discretization. As the time discretization, we employ the convolution quadrature method based on the 2-stage Radau IIA method, for $N_j = 8 \cdot 2^j$ for $j = 0, ..., 7$. The numerical approximations are compared with a reference solution obtained by the same discretization, that has been computed with $h = 2^{-4}$, which corresponds to a boundary element space of 12534 degrees of freedom, and $N = 2048$ time steps.

3.8.2 Scattering from two cubes: Visualization of the numerical solution

In the second experiment, we choose the union of two unit cubes, separated by a gap of length $l = 0.5$, as the interior domain Ω^-. The plane wave (3.54) illuminates the scatterers, and $c = 100$. Figure 3.3 depicts the approximation of the total wave, evaluated in the $y = 0.5$ plane, which cuts through the middle of the cubes, at several time points. The scheme has been used with a $0 - th$ order Raviart–Thomas boundary element discretization with 11088 degrees of freedom and the convolution quadrature time discretization based on the 2–stage Radau IIA method with $N = 2096$ time steps.

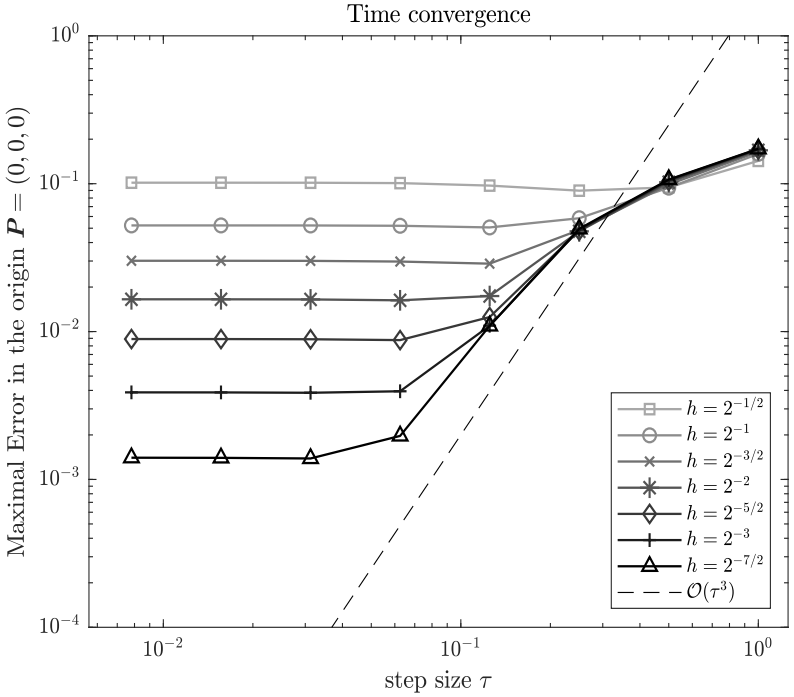

Figure 3.1: Time convergence plot of the fully discrete system for a spherical scatterer, for 0th order Raviart–Thomas boundary elements and the 2-stage Radau IIA based Runge–Kutta convolution quadrature method.

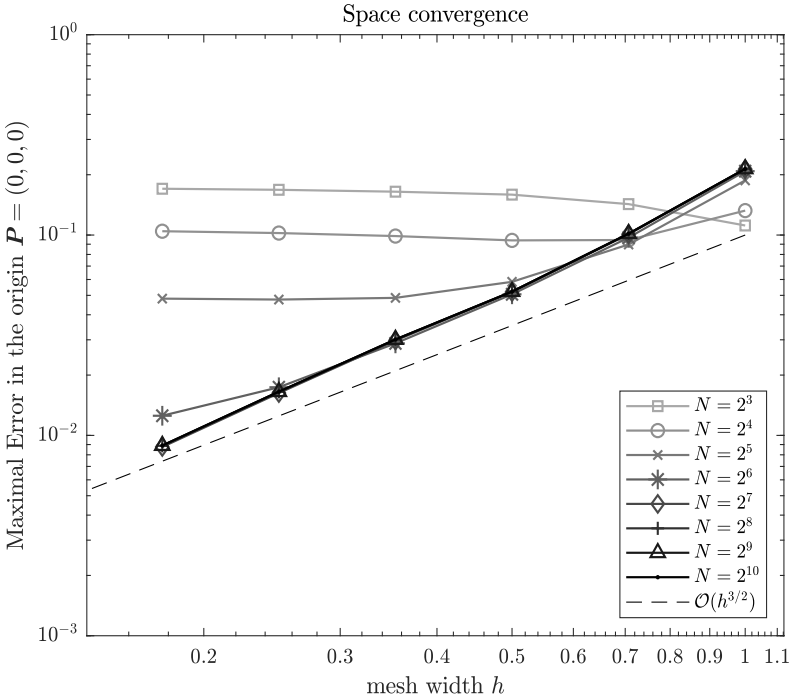

Figure 3.2: Space convergence plot of the fully discrete system for a spherical scatterer, for 0th order Raviart–Thomas boundary elements and the 2-stage Radau IIA based Runge–Kutta convolution quadrature method.

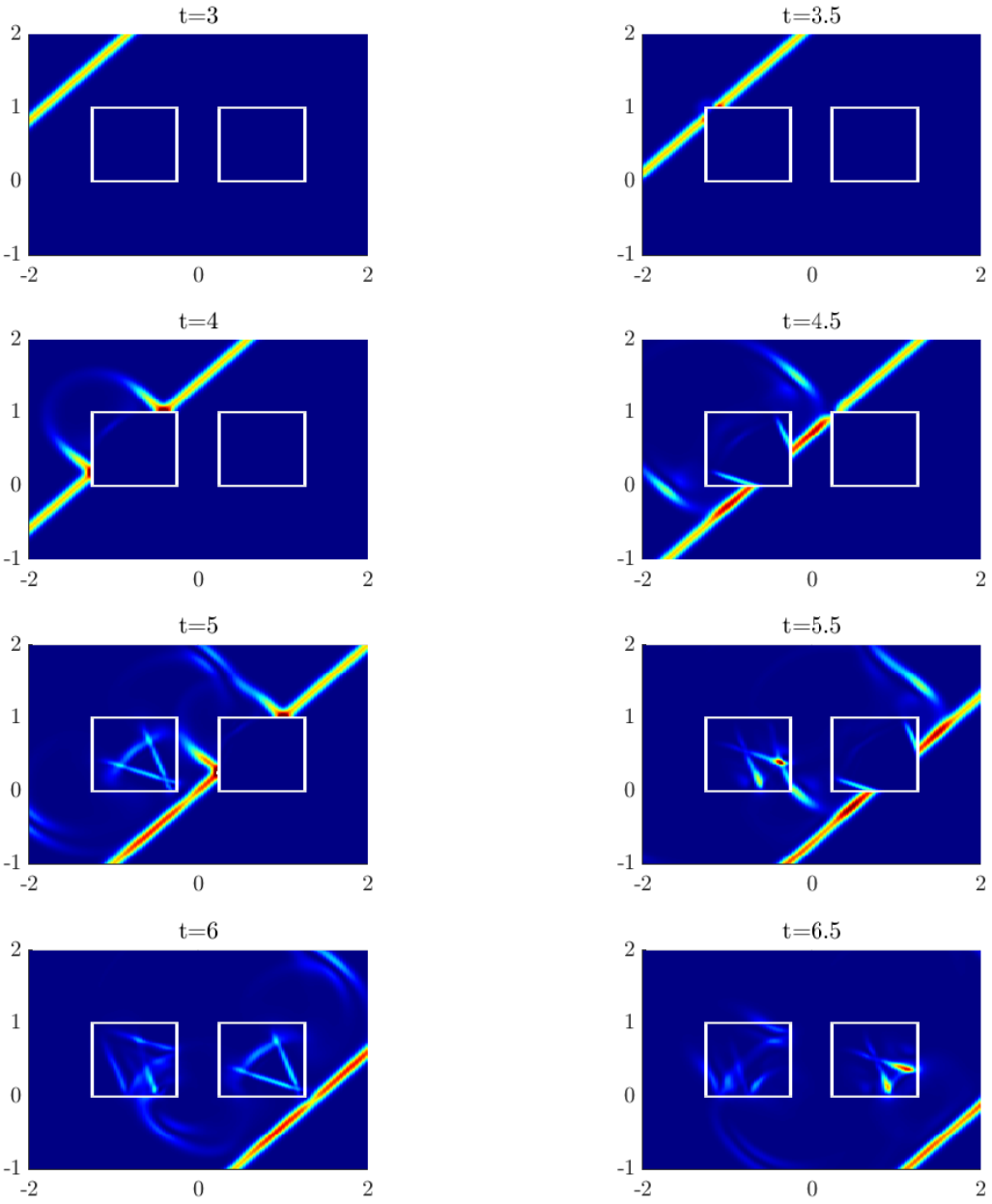

Figure 3.3: Scattering from two cubes, where the time-fractional material law determined by (3.55) is enforced.

CHAPTER 4

An implicit-explicit time discretization scheme for second-order semilinear wave equations with a nonlocal material law and kinetic boundary conditions

The content of this chapter is submitted as [32]. The authors are Selina Burkhard, Marlis Hochbruck and Malik Scheifinger.

In this chapter we construct and analyze an implicit-explicit (IMEX) scheme for the semilinear viscoacoustic wave equation with a retarded material law. It contains a convolution term with exponential kernels and is thus nonlocal in time. Furthermore, the wave equation is equipped with kinetic boundary conditions. We treat the convolution term via additional variables. In order to make the problem well-posed, it is essential to perform an appropriate shift to derive auxiliary differential equations which are coupled to the first–order formulation of the wave equation. For the kinetic boundary conditions, we consider these equations in weighted bulk-surface Sobolev spaces. Second–order error bounds in time are proven for the IMEX scheme and are supported by numerical experiments, where the IMEX scheme is combined with an isoparametric finite element discretization in space.

4.1 Introduction

In this paper, we consider the viscoacoustic wave equation with a convolution term of the form

$$\partial_{tt}u(t) - c^2\Delta u(t) + \int_{-\infty}^{t} b(t-\theta)\Delta u(\theta)\,\mathrm{d}\theta = f(t,u), \qquad u(0) = u_0, \quad u_t(0) = v_0, \tag{4.1a}$$

in a domain $\Omega \subset \mathbb{R}^d$ with smooth boundary Γ and we set $u(\theta) = u_0$ for $\theta < 0$. The viscoacoustic wave equation can be seen as a simplified model of the viscoelastic wave equation. The convolutionary memory term is determined by physical properties and describes the viscosity of the material. It makes the equation nonlocal in time, which is numerically challenging. Here, we study convolution kernels given by a linear combination of exponentials,

$$b(t) = \sum_{j=1}^{m} \beta_j \mathrm{e}{-\lambda_j t}, \qquad \beta_j, \lambda_j > 0. \tag{4.1b}$$

This model that can be found in geophysical literature, e.g., [34, Chap. 2] and more specific in seismology [68]. The model problem using exponential kernels describes the case that most recent history has more influence on the materials reaction and diminishes in the past further away, cf. [34, Sec. 2.1.1]. We say, the material has a fading memory. In mechanical modeling this is used for the standard linear solid, where λ^{-1} is the relaxation time, cf. [101, p. 32]. We assume that the material properties do not change over time, cf. [34]. The kernels (4.1b) are of a special form, which enables us to derive additional auxiliary differential equations, which are coupled to the wave equation. For more general kernels, one can consider convolution quadrature, see e.g., [14, 27, 96, 97, 100, 107, 111].

To complement equation (4.1), we impose appropriate boundary conditions. In particular, we consider both Dirichlet and kinetic boundary conditions in a general framework. The latter are a special kind of dynamic boundary conditions, which take the form of another differential equation posed on the boundary. In two dimensions, kinetic boundary conditions admit the physical interpretation of a vibrating membrane with boundary mass density exposed to linear tension, see [54, Sec. 5&6], [91, p.56]; An example is the membrane of a bass drum which has a hole in the interior that has a thick border, cf. [107, Sec. 3.2]. In [54, 82], dynamic boundary conditions are considered for modeling heat conduction, where heat is created on the boundary.

For the time integration of (4.1) we employ a new implicit-explicit scheme in order to solve the stiff linear part implicitly and we avoid solving a nonlinear system in each step by treating the inhomogeneity explicitly. Due to the smooth boundary we combine this with a nonconforming space discretization with isoparametric finite elements.

In [129, 130] there are analytical results of wave equations with dynamic boundary conditions. In [4], the authors show wellposedness of a parabolic equation with dynamic boundary conditions. Other authors have investigated numerics for kinetic boundary conditions. Examples are [72, 73, 76] for linear and semilinear equations without nonlocal materials. A bulk-surface splitting method is proposed in [5].

The authors of [80] consider the viscoelastic wave equation and simulate its solution using a symmetric interior penalty discontinuous Galerkin method. In [43], space-time methods are used for the linear viscoacoustic equation. Several authors have investigated the viscoelastic or viscoacoustic wave equation as an inverse problem. Examples are [120], [1] with a finite difference method, and [22]. The goal of the last paper is a full wave form inversion of the viscoacoustic wave equation in a div-grad first-order

formulation. The viscoelastic wave equation with standard boundary conditions is considered in [27] for several models. The authors show plots of the displacement function, using convolution quadrature and the finite element method. Furthermore, space-time plots are shown. However, this paper did not focus on the error analysis.

The literature on wave equations with auxiliary differential equations mostly deals with the analysis and stability including a different variable and possibly a delay term, cf. [2]. In [102], promising experiments for the viscoelastic wave equation with a nonlinear stress-strain relation are shown. For the numerical simulation, the ADE system of equations is discretized in time using a second order semi-implicit scheme. It is combined with a second-order time-stepping algorithm and a fourth-order staggered grid finite difference spatial discretization. However, the authors did not provide an error analysis.

There is a broad literature on implicit-explicit (IMEX) schemes, e.g., [52, 81, 92, 116]. The authors of [45] propose an IMEX scheme combined with multiscale methods. A Crank-Nicolson-leapfrog IMEX scheme was constructed in [88, 89]. However, the schemes therein are not equivalent to our IMEX scheme.

The author of [50, 51] considers a related problem to (4.1), where the solution to a Maxwell system with exponential non-locality is approximated. However, in the setting there, the nonlocality is a bounded perturbation, which is not applicable in our situation.

The main contribution of this paper is the construction and the rigorous error analysis of a new IMEX scheme for a wave equation that has a nonlocality in time and is equipped with dynamic boundary conditions. In contrast to the setting in [77], the block structure of the operator in the first-order formulation has at least three components, which is why the calculations here are more involved than in [77]. In particular, we first derive a framework using weighted Sobolev spaces suitable for the wellposedness as well as for the error analysis. Moreover, defining the auxiliary variables is not straight forward, since an appropriate shift has to be included, cf. [2]. Finally, we show a uniform second-order error bound for the time discretization.

In this paper, for the sake of presentation, we do not carry out the full discretization, since it can be done along the lines of [77].

Outline of the paper

In Section 4.2, we state the problem, introduce auxiliary variables and the corresponding system of differential equations and investigate the wellposedness. In Section 4.3, we construct and analyze the numerical approximation by an implicit-explicit (IMEX) scheme in time. We conclude with numerical examples in Section 4.4.

Notation

For the partial derivative with respect to time we use the notation $\partial_t u = u' = u_t$. In this paper, we will consider (4.1a) with Dirichlet boundary conditions (D) or with kinetic boundary conditions (K). This will require different spaces, as defined next. We introduce the following bulk-surface Sobolev spaces,

$$H^k(\Omega,\Gamma) = \left\{ v \in H^k(\Omega) \,\middle|\, \gamma_D(v) \in H^k(\Gamma) \right\}, \quad k \geq 1,$$

of $H^k(\Omega)$-functions with $H^k(\Gamma)$-traces, where γ_D denotes the Dirichlet trace operator, cf. [82]. We further equip $H^k(\Omega,\Gamma)$ with the scalar product, which induces the norm

$$\|v\|^2_{H^k(\Omega,\Gamma)} = \left\|H^k(\Omega)\right\|^2_v + \|\gamma_D(v)\|^2_{H^k(\Gamma)}\,.$$

We denote the spaces

$$H = \begin{cases} L^2(\Omega), & \text{for (D)} \\ L^2(\Omega)\times L^2(\Gamma), & \text{for (K)} \end{cases} \quad \text{and} \quad V = \begin{cases} H^1_0(\Omega), & \text{for (D)} \\ H^1(\Omega,\Gamma), & \text{for (K)} \end{cases}. \tag{4.2a}$$

In [72, Cor. 6.7] it is shown, that $H^1(\Omega,\Gamma)$ is dense in $L^2(\Omega)\times L^2(\Gamma)$ and $C^\infty(\overline{\Omega})$ is dense in $H^1(\Omega,\Gamma)$.

We will make use of weighted spaces. Let V be a Hilbert space as defined in (4.2a) with scalar product $\langle\cdot,\cdot\rangle$, then we define the weighted Hilbert space V_α for some $\alpha>0$ as the space V combined with the weighted scalar product, i.e.,

$$\big(V_\alpha,(\cdot,\cdot)\big), \qquad \text{where} \quad (x,y)\mapsto \alpha\langle x,y\rangle \quad \text{for} \quad x,y\in V.$$

Let Γ be C^1-regular. For a function $v\in H^1(\Omega)$ and the outer unit normal vector $\boldsymbol{n}$, we define the surface gradient

$$\nabla_\Gamma v = (\partial_{j,\Gamma} v)_{j=1}^d = (I-\boldsymbol{n}\boldsymbol{n}^T)\nabla v$$

and the Laplace-Beltrami operator

$$\Delta_\Gamma v = \sum_{j=1}^d \partial^2_{j,\Gamma} v.$$

For the weak formulation of our PDEs we will make use of the well-known Gauss theorem, which also holds for the above surface operators, see also [82, p. 111],

$$\begin{aligned} -\int_\Omega (\Delta u)\varphi\,\mathrm{d}x &= \int_\Omega \nabla u\nabla\varphi\,\mathrm{d}x - \int_\Gamma (\boldsymbol{n}\cdot\nabla u)\varphi\,\mathrm{d}x, \\ -\int_\Gamma (\Delta_\Gamma u)\varphi\,\mathrm{d}x &= \int_\Gamma \nabla_\Gamma u\nabla_\Gamma\varphi\,\mathrm{d}x. \end{aligned}$$

4.2 Analytical framework

Throughout this paper, we consider (4.1a) with Dirichlet boundary conditions as well as kinetic boundary conditions. In this section, we describe the framework for the two types of boundary conditions and how both cases will be handled in the further course of this paper. We will derive auxiliary differential equations for the treatment of the convolution and investigate its wellposedness by means of evolution equations in suitable spaces.

4.2.1 Problem statement

We assume Γ to be the smooth boundary of the domain $\Omega \subset \mathbb{R}^d$ and impose kinetic boundary conditions, i.e.,

$$\begin{aligned} &\partial_{tt}u(t) - c^2\Delta u(t) + \int_{-\infty}^{t} b(t-s)\Delta u(s)\,\mathrm{d}s = f_\Omega(t), \\ &\partial_{tt}u(t) - c^2\Delta_\Gamma u(t) + c^2\boldsymbol{n}\cdot\nabla u + \int_{-\infty}^{t} b(t-s)\Delta_\Gamma u(s)\,\mathrm{d}s \\ &\qquad\qquad - \int_{-\infty}^{t} b(t-s)\boldsymbol{n}\cdot\nabla u(s)\,\mathrm{d}s = f_\Gamma(t) \\ &u(0) = u_0, \quad \partial_t u(0) = v_0, \end{aligned} \tag{4.4}$$

where we again set $u(s) = u_0$ for $s < 0$. In order to abbreviate the notation, we further define the extended Laplace operator

$$\Delta_{\Omega,\Gamma} = \begin{cases} \Delta, & \text{in} \quad \Omega, \\ \Delta_\Gamma - \boldsymbol{n}\cdot\nabla, & \text{on} \quad \Gamma. \end{cases}$$

Note that for $u \in H_0^1(\Omega)$, the extended Laplace operator only acts on the inner domain. Then, (4.1a) with Dirichlet or kinetic boundary conditions can be summarized as

$$\partial_{tt}u(t) - c^2\Delta_{\Omega,\Gamma}u(t) + \int_{-\infty}^{t} b(t-s)\Delta_{\Omega,\Gamma}u(s)\mathrm{d}s = f(t). \tag{4.5}$$

4.2.2 Auxiliary differential equations

In this subsection we derive auxiliary differential equations for the treatment of the convolution in (4.5) and investigate its wellposedness in the setting of an evolution equation. Following [2], we perform a shift of the variable in the convolution term and obtain

$$\int_{-\infty}^{t} \beta_j \mathrm{e}^{-\lambda_j(t-\theta)}\Delta_{\Omega,\Gamma}u(\theta)\,\mathrm{d}\theta = \frac{\beta_j}{\lambda_j}\Delta_{\Omega,\Gamma}u(t) - \beta_j\Delta_{\Omega,\Gamma}M_j(t), \quad j = 1,\dots,m,$$

with the auxiliary variables

$$M_j(t) = \int_{-\infty}^{t} \mathrm{e}^{-\lambda_j(t-\theta)}\big(u(t) - u(\theta)\big)\,\mathrm{d}\theta, \qquad t \geq 0.$$

We introduce the notation

$$M = (M_j)_{j=1}^m, \quad \beta = (\beta_j)_{j=1}^m, \quad \mathbf{1} = (1)_{j=1}^m, \quad \Lambda = \mathrm{diag}(\lambda_1,\dots,\lambda_m).$$

Then, we obtain the following first-order in time coupled PDE system for (4.5)

$$\begin{aligned} \partial_t u &= v, & u(0) &= u_0, \\ \partial_t v &= \alpha\Delta_{\Omega,\Gamma} u + \Delta_{\Omega,\Gamma}\beta^T M + f, & v(0) &= v_0, & \alpha &= c^2 - \sum_{j=1}^m \frac{\beta_j}{\lambda_j}, \\ \partial_t M_j &= -\lambda_j M_j + \frac{1}{\lambda_j} v, & M_j(0) &= 0, & j &= 1,\dots,m. \end{aligned}$$

In a compact form, (4.6) can be written as

$$x' + \mathcal{A}x = F, \tag{4.7a}$$

where

$$x = \begin{pmatrix} u \\ v \\ M \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} 0 & -\mathrm{I} & 0 \\ -\alpha\Delta_{\Omega,\Gamma} & 0 & -\beta\otimes\Delta_{\Omega,\Gamma} \\ 0 & -\Lambda^{-1}\mathbf{1} & \Lambda \end{pmatrix}, \quad F = \begin{pmatrix} 0 \\ f \\ 0 \end{pmatrix}. \tag{4.7b}$$

Remark 4.1. In applications, we often know the Laplace transformation B rather than the kernel b itself, see, e.g., [34, 68]. The Laplace transform of the differential equation (4.1) with frequency variable $s \in \mathbb{C}$ is given as

$$\big(s^2 - (c^2 - B(s))\Delta_{\Omega,\Gamma}\big)U(s) = F(s), \qquad B(s) = \sum_{j=1}^m \frac{\beta_j}{s+\lambda_j},$$

where $U(s), F(s)$ denote the Laplace transformations of u, f, respectively. Since $-\Delta_{\Omega,\Gamma}$ is a positive semidefinite operator, assuming

$$\alpha = c^2 - \sum_{j=1}^m \frac{\beta_j}{\lambda_j} > 0 \tag{4.8}$$

is sufficient to ensure that, for a given $F(s)$, this equation has a unique solution $U(s)$ for all $\operatorname{Re} s = \sigma > 0$. Hence we assume (4.8) in the remaining manuscript.

4.2.3 Wellposedness

Next we consider the wellposedness of the coupled PDE system (4.6) for Dirichlet (D) and for kinetic (K) boundary conditions. We will show that, in both cases, $\mathcal{A}$ generates a monotone operator on the respective Hilbert space

$$X = V_\alpha \times H \times \bigtimes_{j=1}^m V_{\mu_j} \tag{4.9}$$

with V_α defined in (4.2) for $\alpha > 0$ and $\mu_j = \beta_j\lambda_j > 0$. In particular, $\mathcal{A}$ is monotone, i.e.,

$$(\mathcal{A}x, x)_X \geq -\mathrm{c}_m \|x\|_X 2 \qquad \text{for all} \quad x \in X, \tag{4.10}$$

cf. [91, Assumption 2.3]. For Dirichlet boundary conditions, we have $c_m = 0$, which means that $\mathcal{A}$ generates a contractive semigroup, while for kinetic boundary conditions, (4.10) holds for

$$\mathrm{c}_m > \frac{1}{2}, \qquad \mathrm{c}_m > \frac{\alpha + \mathbf{1}^T\beta}{2}, \qquad \lambda_j \mathrm{c}_m > \frac{1}{2} - \lambda_j^2, \qquad j = 1,\dots,m. \tag{4.11}$$

Theorem 4.2. *Let $\mathcal{A}$ and x be given as in (4.7b), describing the first-order formulation of (4.5).*

(D) The operator $-\mathcal{A}$ with domain

$$\mathcal{D}(\mathcal{A}) = \left\{ x \in H_0^1(\Omega)^{m+2} \,\middle|\, \alpha u + \beta^T M \in H^2(\Omega) \right\}$$

(K) For c_m chosen such that (4.11) holds, the shifted operator $-(\mathcal{A} + \mathrm{c}_m \mathrm{I})$ with domain

$$\mathcal{D}(\mathcal{A} + \mathrm{c}_m \mathrm{I}) = \left\{ x \in H^1(\Omega, \Gamma)^{m+2} \,\middle|\, \alpha u + \beta^T M \in H^2(\Omega, \Gamma) \right\}$$

generates a contractive C_0-semigroup on X defined in (4.9).

In order to obtain local wellposedness of (4.7a) we make the following assumption on the inhomogeneity.

Assumption 4.3. *[77, Assumption 4.1] Let $\Theta \in \{\Omega, \Gamma\}$.*

(a) *The inhomogeneities $f = f_\Theta$, in (4.4) satisfy*

$$f_\Theta \in C^1([0,T] \times \overline{\Theta} \times \mathbb{R}; \mathbb{R})$$

and can be split into

$$f(t,\xi,u) = f_1(t,\xi) + f_2(\xi,u) \quad \text{or} \quad f(t,\xi,u) = f_1(t,\xi) + f_2(t,u).$$

(b) *Furthermore, we assume the growth conditions, that there exist*

$$\zeta_\Omega \begin{cases} < \infty, & d = 2, \\ \leq \frac{d}{d-2} & d \geq 3, \end{cases} \quad \text{and} \quad \zeta_\Gamma \begin{cases} < \infty, & d = 2,3, \\ \leq \frac{d-1}{d-3} & d \geq 4, \end{cases}$$

such that for all $(t,\xi,u) \in [0,T] \times \Theta \times \mathbb{R}$ it holds that

$$|f_\Theta(t,\xi,u)| \leq C(1 + |u|^{\zeta_\Theta}), \qquad |\nabla f_\Theta(t,\xi,u)| \leq C(1 + |u|^{\zeta_\Theta - 1}).$$

Remark 4.4. If Assumption 4.3 holds, then, (4.7a) is locally wellposed, i.e., for every initial value $x_0 \in X$ there exists $t^\star(x_0) > 0$ such that for all $T < t^\star(x_0)$, (4.7a) has a unique solution

$$x \in C^1([0,T], X) \cap C([0,T], \mathcal{D}(\mathcal{A})).$$

The evolution equation (4.7a) fits into the framework of [72, 74, 91].

Proof of Theorem 4.2. For better readability, we only show the proof in the case $m = 1$, i.e., the case of one exponential kernel. We demonstrate the calculations for the wave equation with kinetic boundary conditions, the case of Dirichlet boundary conditions works analogously. Employing the Gauss theorems (4.3), we see that the kinetic boundary condition leads to solving (4.7b) on the space given in (4.9).

We will use the Lumer-Phillips theorem [115, Sec.1.3]. To this end, we show that $\mathcal{A} + \mathrm{c}_m \mathrm{Id}$ is densely defined, monotone, and has full range.

For the monotonicity we calculate by using partial integration (4.3) and Young

$$\begin{aligned}
&(\mathcal{A}x + \mathrm{c}_m x, x)_X \\
=\ & -\alpha\langle v, u\rangle_{L^2(\Omega,\Gamma)} + \mathrm{c}_m\alpha\|\nabla u\|^2_{L^2(\Omega,\Gamma)} + \mathrm{c}_m\alpha\|u\|^2_{L^2(\Omega,\Gamma)} + \mathrm{c}_m\|v\|^2_{L^2(\Omega,\Gamma)} \\
&+ \beta\lambda^2\|\nabla M\|^2_{L^2(\Omega,\Gamma)} + \beta\lambda^2\|M\|^2_{L^2(\Omega,\Gamma)} - \beta\langle v, M\rangle_{L^2(\Omega,\Gamma)} \\
&+ \mathrm{c}_m\mu\|\nabla M\|^2_{L^2(\Omega,\Gamma)} + \mathrm{c}_m\mu\|M\|^2_{L^2(\Omega,\Gamma)} \\
\geq\ & -\frac{\alpha}{2}\left(\|v\|^2_{L^2(\Omega,\Gamma)} + \|u\|^2_{L^2(\Omega,\Gamma)}\right) - \frac{\beta}{2}\left(\|v\|^2_{L^2(\Omega,\Gamma)} + \|M\|^2_{L^2(\Omega,\Gamma)}\right) \\
&+ \mathrm{c}_m\|v\|^2_{L^2(\Omega,\Gamma)} + \mathrm{c}_m\alpha\|u\|^2_{L^2(\Omega,\Gamma)} + \beta\lambda^2\|M\|^2_{L^2(\Omega,\Gamma)} + \mathrm{c}_m\mu\|M\|^2_{L^2(\Omega,\Gamma)} \\
=\ & \alpha\|u\|^2_{L^2(\Omega,\Gamma)}\left(\mathrm{c}_m - \frac{1}{2}\right) + \|v\|^2_{L^2(\Omega,\Gamma)}\left(\mathrm{c}_m - \frac{\alpha+\beta}{2}\right) + \|M\|^2_{L^2(\Omega,\Gamma)}\left(\mathrm{c}_m\mu - \frac{\beta}{2} + \beta\lambda^2\right) \\
\geq\ & 0.
\end{aligned}$$

To show that $\mathcal{A}$ has full range, let $\gamma > \mathrm{c}_m$, $y := (f, g, h) \in X$. We claim that there exists $x := (u, v, M) \in \mathcal{D}(\mathcal{A})$ such that $(\gamma + \mathcal{A})x = y$

$$\gamma u = v + f, \tag{4.12a}$$

$$\gamma v = \alpha\Delta_{\Omega,\Gamma}u + \beta\Delta_{\Omega,\Gamma}M + g, \tag{4.12b}$$

$$\gamma M = -\lambda M + \frac{1}{\lambda}v + h. \tag{4.12c}$$

We aim to insert

$$u = \frac{1}{\gamma}(v + f), \qquad M = \frac{1}{\gamma+\lambda}(\frac{1}{\lambda}v + h)$$

into (4.12b) and solve for v. To do so, we use the operator

$$\Delta_{\Omega,\Gamma} : H^1(\Omega,\Gamma) \to H^{-1}(\Omega,\Gamma)$$

for the moment. Then, we have to solve

$$\gamma v = \frac{\alpha}{\gamma}\Delta_{\Omega,\Gamma}(v + f) + \frac{\beta}{\gamma+\lambda}\Delta_{\Omega,\Gamma}(\frac{1}{\lambda}v + h) + g$$

which is equivalent to

$$v - \frac{1}{\gamma}(\frac{\alpha}{\gamma} + \frac{\beta}{\lambda(\gamma+\lambda)})\Delta_{\Omega,\Gamma}v = \frac{\alpha}{\gamma^2}\Delta_{\Omega,\Gamma}f + \frac{\beta}{\gamma(\gamma+\lambda)}\Delta_{\Omega,\Gamma}h + \frac{1}{\gamma}g. \tag{4.13}$$

The weak formulation is given as: find $v \in H^1(\Omega,\Gamma)$ such that

$$\begin{aligned}
&\langle v, \varphi\rangle_{L^2(\Omega,\Gamma)} + \frac{1}{\gamma}(\frac{\alpha}{\gamma} + \frac{\beta}{\lambda(\gamma+\lambda)})\langle\nabla v, \nabla\varphi\rangle_{L^2(\Omega,\Gamma)} \\
=& -\frac{\alpha}{\gamma^2}\langle\nabla f, \nabla\varphi\rangle_{L^2(\Omega,\Gamma)} - \frac{\beta}{\gamma(\gamma+\lambda)}\langle\nabla h, \nabla\varphi\rangle_{L^2(\Omega,\Gamma)} + \frac{1}{\gamma}\langle g, \varphi\rangle_{L^2(\Omega,\Gamma)},
\end{aligned}$$

for all $\varphi \in H^1(\Omega,\Gamma)$. By the Lax–Milgram theorem we obtain a unique solution $v \in H^1(\Omega,\Gamma)$ of (4.13). Inserting this solution into (4.12a) and (4.12c) gives us $u, M \in H^1(\Omega,\Gamma)$ such that

$$\alpha\Delta_{\Omega,\Gamma}u + \beta\Delta_{\Omega,\Gamma}M = \frac{\alpha}{\gamma}\Delta_{\Omega,\Gamma}(v + f) + \frac{\beta}{\gamma+\lambda}\Delta_{\Omega,\Gamma}(\frac{1}{\lambda}v + h)$$

In order to make sure, that $x = (u, v, M) \in \mathcal{D}(\mathcal{A})$, we test the above equation with $\varphi \in H^1(\Omega, \Gamma)$ which yields

$$\begin{aligned}\langle \nabla(\alpha u + \beta M), \nabla\varphi\rangle_{L^2(\Omega,\Gamma)} &= \frac{\alpha}{\gamma}\langle \nabla(v + f), \nabla\varphi\rangle_{L^2(\Omega,\Gamma)} + \frac{\beta}{\gamma+\lambda}\langle \nabla(\frac{1}{\lambda}v + h), \nabla\varphi\rangle_{L^2(\Omega,\Gamma)} \\ &= \langle g - \gamma v, \varphi\rangle_{L^2(\Omega,\Gamma)},\end{aligned}$$

and using $g \in L^2(\Omega, \Gamma)$ and $v \in H^1(\Omega, \Gamma)$ shows $x = (u, v, M) \in \mathcal{D}(\mathcal{A})$.

Note that the full range of $\gamma + \mathcal{A}$ was shown for arbitrary $\gamma > c_m$. The fact that $\mathcal{A}$ is densely defined therefore follows by [125, Prop. I.4.2]. □

4.3 Time discretization – implicit-explicit scheme

In this section, we introduce the IMEX scheme for the time discretization of the solution to (4.1a) and its properties.

4.3.1 Construction of the IMEX scheme

Following [77], we set up the IMEX scheme as a perturbation of the Crank-Nicolson scheme. The latter one computes $x^n \approx x(t_n)$ for $t_n = n\tau$, where $\tau > 0$ denotes the step size via

$$x^{n+1} = x^n + \frac{\tau}{2}\big(-\mathcal{A}(x^n + x^{n+1}) + F^n + F^{n+1}\big),$$

where

$$F^n = \begin{pmatrix} 0 \\ f^n \\ 0 \end{pmatrix}, \qquad \text{and} \qquad f^n = f(t_n, u^n). \tag{4.14a}$$

Equivalently we can write this as

$$R_+ x^{n+1} = R_- x^n + \frac{\tau}{2}\big(F^n + F^{n+1}\big), \qquad R_\pm = \mathrm{Id} \pm \frac{\tau}{2}\mathcal{A}. \tag{4.15}$$

With the parameters β_j and λ_j of the convolution kernel (4.1b), we define the following scalars, which will be used in the discretization of the differential equation of M,

$$\gamma_{j,\pm} = 1 \pm \frac{\tau\lambda_j}{2}, \qquad \gamma_j = \frac{\gamma_{j,-}}{\gamma_{j,+}}.$$

Furthermore, we introduce a modification of the matrix Λ as

$$\widetilde{\Lambda} = \mathrm{diag}(\lambda_1\gamma_{1,+}, \dots, \lambda_m\gamma_{m,+}), \tag{4.16}$$

and the modified scalars

$$\widetilde{\alpha} = \alpha + \beta^T\widetilde{\Lambda}^{-1}\mathbf{1} = \left(\alpha + \sum_{j=1}^{m}\frac{\beta_j}{\lambda_j\gamma_{j,+}}\right) > \alpha. \tag{4.17}$$

We further introduce the notation

$$\widetilde{\beta} = \frac{1}{2}\big(\beta_1(1+\gamma_1), \dots, \beta_m(1+\gamma_m)\big), \tag{4.18}$$

and note that $\beta_j(1+\gamma_j)/2 \in [0, \beta_j)$ for $j = 1, \dots, m$.

Similarly to [77, Lem. 2.5] it can be shown that with $j = 1, \dots, m$ and f^n defined in (4.14a), the Crank-Nicolson scheme (4.14) is equivalent to

$$\begin{aligned}
u^{n+1} &= u^n + \tau v^{n+\frac{1}{2}},\\
v^{n+\frac{1}{2}} &= v^n + \frac{\tau}{2}\alpha\Delta_{\Omega,\Gamma}u^n + \frac{\tau}{2}\Delta_{\Omega,\Gamma}\widetilde{\beta}^T M^n + \frac{\tau^2}{4}\widetilde{\alpha}\Delta_{\Omega,\Gamma}v^{n+\frac{1}{2}} + \frac{\tau}{4}(f^n + f^{n+1}),\\
M_j^{n+1} &= \gamma_j M_j^n + \gamma_{j,+}^{-1}\frac{\tau}{\lambda_j}v^{n+\frac{1}{2}},\\
v^{n+1} &= v^{n+\frac{1}{2}} + \frac{\tau}{2}\alpha\Delta_{\Omega,\Gamma}u^n + \frac{\tau}{2}\Delta_{\Omega,\Gamma}\widetilde{\beta}^T M^n + \frac{\tau^2}{4}\widetilde{\alpha}\Delta_{\Omega,\Gamma}v^{n+\frac{1}{2}} + \frac{\tau}{4}(f^n + f^{n+1}).
\end{aligned}$$

If the right hand side f is nonlinear, we will have to solve a nonlinear system in each step of the Crank-Nicolson scheme, which is very expensive. To overcome this difficulty, we use the IMEX scheme instead. The idea of the IMEX scheme is to treat the stiff linear part implicitly and the non-stiff non-linear part explicitly, such that the solution of one linear system of equations in each time step is sufficient.

Following [77, Section 2.2.], we derive the scheme via a combination of the Crank-Nicolson and with the leapfrog scheme and, with $j = 1, \dots, m$, arrive at

$$v^{n+\frac{1}{2}} = v^n + \frac{\tau}{2}\alpha\Delta_{\Omega,\Gamma}u^n + \frac{\tau}{2}\Delta_{\Omega,\Gamma}\widetilde{\beta}^T M^n + \frac{\tau^2}{4}\widetilde{\alpha}\Delta_{\Omega,\Gamma}v^{n+\frac{1}{2}} + \frac{\tau}{2}f^n, \tag{4.19a}$$

$$\begin{aligned}
u^{n+1} &= u^n + \tau v^{n+\frac{1}{2}},\\
M_j^{n+1} &= \gamma_j M_j^n + \gamma_{j,+}^{-1}\frac{\tau}{\lambda_j}v^{n+\frac{1}{2}},
\end{aligned}$$

$$v^{n+1} = v^{n+\frac{1}{2}} + \frac{\tau}{2}\alpha\Delta_{\Omega,\Gamma}u^n + \frac{\tau}{2}\Delta_{\Omega,\Gamma}\widetilde{\beta}^T M^n + \frac{\tau^2}{4}\widetilde{\alpha}\Delta_{\Omega,\Gamma}v^{n+\frac{1}{2}} + \frac{\tau}{2}f^{n+1}. \tag{4.19b}$$

An equivalent way to compute v^{n+1} is obtained by subtracting (4.19a) and (4.19b) as

$$v^{n+1} = -v^n + 2v^{n+1/2} + \frac{\tau}{2}(f^{n+1} - f^n),$$

see also [77, Remark 2.6]. In the scheme (4.19), the nonlinearity f is treated explicitly.

4.3.2 Wellposedness and reformulation of the IMEX scheme

To prove wellposedness of the IMEX scheme define the operators

$$Q_\pm = I \pm \big(-\frac{\tau^2}{4}\widetilde{\alpha}\Delta_{\Omega,\Gamma}\big), \tag{4.20}$$

with weak formulation: for given $z \in V$ find $y \in H$ such that

$$\langle z, w\rangle_H \pm \langle \nabla z, \nabla w\rangle_H = \langle y, w\rangle_H \quad \text{for all} \quad w \in V,$$

we define $y = Q_\pm z$. With this notation, we can characterize the half step $v^{n+\frac{1}{2}}$ via

$$Q_+ v^{n+\frac{1}{2}} = v^n + \frac{\tau}{2}\Delta_{\Omega,\Gamma}\big(\alpha u^n + \widetilde{\beta}^T M^n\big) + \frac{\tau}{2}f^n.$$

For our error analysis we will use bounds on the operators $Q_\pm$ using the spaces defined in (4.2a). Up to the weighting constants the following lemma was given in [77, Lemma 2.7].

Lemma 4.5. *Let $Q_\pm$ be defined as in (4.20) with $\widetilde{\alpha}$ as in (4.17). Then $Q_+ : \mathcal{D}(\Delta_{\Omega,\Gamma}) \to H$ is invertible and we have*

$$\left\| \frac{\tau^2}{4} \widetilde{\alpha} \Delta_{\Omega,\Gamma} Q_+^{-1} \right\|_{H \leftarrow H} \leq 1, \tag{4.21a}$$

where $\|\cdot\|_{H\leftarrow H}$ denotes the operator norm. Furthermore, for $\tau > 0$ in case (D) and $0 < \tau < \sqrt{\frac{2}{\widetilde{\alpha}}}$ in case (K), we have the bounds

$$\begin{aligned} \left\|Q_+^{-1}\right\|_{V\leftarrow H} &\leq \frac{1}{\tau}\sqrt{\frac{2}{\widetilde{\alpha}}}, \\ \left\|Q_- Q_+^{-1}\right\|_{H\leftarrow H} &\leq \mathrm{e}^{\frac{\tau^2}{2}}. \end{aligned} \tag{4.21b}$$

Employing the invertibility of Q_+ we obtain wellposedness of the IMEX scheme as in [91, Cor. 4.7] and [77, Cor. 2.8].

Lemma 4.6. *The IMEX scheme is wellposed. We define $\widehat{\beta} = (\widehat{\beta}_j)_{j=1}^m$ with $\widehat{\beta}_j \in [-\beta_j, \beta_j]$. Then for initial values $u^0, v^0 \in V$ and $M^0 = \mathbf{0}_m$, we have for $j = 1, \dots, m$ that*

$$u^n, M_j^n \in V, \quad v^{n+\frac{1}{2}} \in \mathcal{D}(\Delta_{\Omega,\Gamma}), \quad v^{n+1} \in H, \quad \Delta_{\Omega,\Gamma}(\alpha u^n + \widehat{\beta}^T M^n) \in H.$$

Proof. As in [77, Cor. 2.8], the claim is proven by induction over $n \in \mathbb{N}_0$. Due to $M_j^0 = 0$, the statement is true for $n = 0$. Then, exploiting the fact that $\widetilde{\beta}_j \in [0, \beta_j)$ for each $j = 1, \dots, m$, such that $\alpha\Delta_{\Omega,\Gamma} u^n + \Delta_{\Omega,\Gamma}\widetilde{\beta}^T M^n \in H$, the claim follows. □

We derive an equivalent first–order formulation for the IMEX scheme, cf. [91, Lemma 4.8] and [77, Lemma 2.10], where we make use of the notation introduced in (4.16) and (4.18).

Lemma 4.7. *Let $\tau \mathrm{c}_m < 2$ and if we have kinetic boundary conditions let $\tau < \sqrt{\frac{2}{\widetilde{\alpha}}}$. Then, the matrix R_+ from (4.15) is invertible and, with $S_+ = Q_+^{-1}\Delta_{\Omega,\Gamma}$ and $R = R_+^{-1}R_-$ we have*

$$R = \begin{pmatrix} 1 + \frac{\tau^2}{2}\alpha S_+ & \tau Q_+^{-1} & \frac{\tau^2}{2}\widetilde{\beta}^T \otimes S_+ \\ \tau\alpha S_+ & Q_- Q_+^{-1} & \tau\alpha\widetilde{\beta}^T \otimes S_+ \\ \frac{\tau^2}{2}\alpha\widetilde{\Lambda}^{-1} \otimes S_+\mathbf{1} & \tau\widetilde{\Lambda}^{-1} \otimes Q_+^{-1}\mathbf{1} & \Lambda + \frac{\tau^2}{2}\big((\widetilde{\Lambda}^{-1}\widetilde{\beta})^T \otimes \mathbf{1}\big) \otimes S_+ \end{pmatrix}$$

and

$$R_+^{-1} = \begin{pmatrix} \mathrm{Id} + \frac{\tau^2}{4}\alpha S_+ & \frac{\tau}{2}Q_+^{-1} & \frac{\tau^2}{4}\beta^T\Lambda\widetilde{\Lambda}^{-1} \otimes S_+ \\ \frac{\tau}{2}\alpha S_+ & Q_+^{-1} & \frac{\tau}{2}\beta^T\Lambda\widetilde{\Lambda}^{-1} \otimes S_+ \\ \frac{\tau^2}{4}\alpha\widetilde{\Lambda}^{-1} \otimes S_+\mathbf{1} & \frac{\tau}{2}\widetilde{\Lambda}^{-1} \otimes Q_+^{-1}\mathbf{1} & \Lambda\widetilde{\Lambda}^{-1} + \frac{\tau^2}{4}\widetilde{\Lambda}^{-1}\mathbf{1}\beta^T\Lambda\widetilde{\Lambda}^{-1} \otimes S_+ \end{pmatrix}.$$

Furthermore, the matrix $R_+^{-1} : X \to \mathcal{D}(\mathcal{A})$ satisfies $\left\|R_+^{-1}\right\| \leq 1$ and R has a continuous extension on X and $\|R\| \leq \mathrm{e}^{\tau \mathrm{c}_m}$.

The IMEX scheme is equivalent to the first-order formulation

$$x^{n+1} = Rx^n + \frac{\tau}{2}R_+^{-1}y^n + \frac{\tau^2}{4}R_+^{-1}z^n,$$

where

$$y^n = \begin{pmatrix} 0 \\ 1 \\ \mathbf{0}_m \end{pmatrix} \otimes (f^n + f^{n+1}), \qquad z^n = \begin{pmatrix} 1 \\ 0 \\ \Lambda^{-1}\mathbf{1} \end{pmatrix} \otimes (f^n - f^{n+1}).$$

Proof. The proof of the invertibility and the bounds follow along the lines of [77, Lemma 2.10] and [72, Lemma 2.14]. For the ease of presentation we only treat the case $m = 1$. A direct calculation shows that R and R_+^{-1} are given as above. Let $x = (u, v, M)^T \in X$ and we will first use $\Delta_{\Omega,\Gamma}$ mapping from V to its dual, this means that $S_+ : V \to V$. Then we have that the components of

$$w \coloneqq R_+^{-1} x$$

are given by

$$\begin{aligned} w_1 &= \big(\mathrm{Id} + \alpha\frac{\tau^2}{4}S_+\big)u + \frac{\tau}{2}Q_+^{-1}v + \frac{\tau^2}{4}\frac{\beta}{\gamma_+}S_+M, \\ w_2 &= \alpha\frac{\tau}{2}S_+u + Q_+^{-1}v + \alpha\frac{\tau}{2}\frac{\beta}{\gamma_+}S_+M, \\ w_3 &= \alpha\frac{\tau}{4\lambda\gamma_+}S_+u + \frac{\tau}{2\lambda\gamma_+}Q_+^{-1}v + \frac{1}{\gamma_+}\big(Q_+^{-1} - \alpha\frac{\tau^2}{4}S_+\big)M, \end{aligned}$$

and lie in V. We further obtain

$$\Delta_{\Omega,\Gamma}\big(\alpha w_1 + \beta w_3\big) = \alpha\Delta_{\Omega,\Gamma}Q_+^{-1}u + \big(\frac{\alpha\tau}{2} + \frac{\beta\tau}{2\lambda\gamma_+}\big)\Delta_{\Omega,\Gamma}Q_+^{-1}v + \frac{\beta}{\gamma_+}\Delta_{\Omega,\Gamma}Q_+^{-1}M \in H,$$

by Lemma 4.5, i.e., we verified that $R_+^{-1} : X \to \mathcal{D}(\mathcal{A})$.

The proof of the equivalence is done analogously to [91, Lemma 4.8]. □

4.3.3 Error analysis of the IMEX scheme

We now turn to the error estimation of the IMEX scheme. The main idea is, that the defect of the IMEX scheme can be written as the defect of the Crank-Nicolson scheme with an additional term. By Assumption 4.3, the inhomogeneity f is locally Lipschitz continuous, i.e., for $\|u\|_V, \|v\|_V \le \rho$ it holds

$$\|f(\cdot,\cdot,u) - f(\cdot,\cdot,v)\|_H \le L_\rho \|u - v\|_V, \qquad L_\rho = C(1 + \rho^{\zeta_\Omega - 1} + \rho^{\zeta_\Gamma - 1}), \tag{4.23}$$

where C is a constant which is independent of ρ.

The following result can be found for the wave equation without retarded material laws in [77], for the more detailed version we reference to [90].

Theorem 4.8 (Error bound IMEX scheme)**.** *Assume that the solution $x = (u, v, M)$ of (4.7) satisfies $u \in C^4([0,T], H) \cap C^3([0,T], V)$ and $x \in C^2([0,T], \mathcal{D}(\mathcal{A}))$ and that $\tau > 0$ is sufficiently small. Then, the approximation $x^n \approx x(t_n)$, $t_n = n\tau$ given in (4.22) satisfies the error bound*

$$\|x^n - x(t_n)\|_X \le C\mathrm{e}^{Kt_n}\tau^2,$$

where $K = \mathrm{c}_m + \frac{L_\rho(1+\sqrt{2})}{\sqrt{\alpha} - L_\rho\tau(1+\sqrt{2})}$ and the constant C only depends on u and T, and L_ρ defined in (4.23).

Proof. For the ease of presentation we only present the case $m = 1$. During this proof we again use a $\sim$ for an exact evaluation, e.g., we write $\widetilde{x}^n = x(t_n)$.

(1) *Error recursion.* Denote the first-order error by

$$e^n = x^n - \widetilde{x}^n.$$

We insert the exact solution into the IMEX scheme (4.22) and obtain as in [91, (4.29)] that

$$\widetilde{x}^{n+1} = R\widetilde{x}^n + \frac{\tau}{2}R_+^{-1}\widetilde{y}^n + \frac{\tau^2}{4}R_+^{-1}\widetilde{z}^n - \delta_{\mathrm{IMEX}}^{n+1}, \tag{4.24}$$

with

$$\delta_{\mathrm{IMEX}}^{n+1} = R_+^{-1}\delta_{\mathrm{CN}}^{n+1} + \widetilde{\delta}^{n+1}, \qquad \widetilde{\delta}^{n+1} = \frac{\tau^2}{4}\begin{pmatrix} 1 \\ \frac{\tau}{2}\widetilde{\alpha}\Delta_{\Omega,\Gamma} \\ \frac{1}{\lambda\gamma_+} \end{pmatrix} \otimes Q_+^{-1}(\widetilde{f}^n - \widetilde{f}^{n+1}) \tag{4.25}$$

and $\delta_{\mathrm{CN}}^{n+1}$ is the defect from the Crank-Nicolson scheme (4.14). As in [91, Thm. 4.3], it can be seen that $\|\delta_{\mathrm{CN}}^{n+1}\|_X \leq C\tau^3$. Substracting (4.24) from (4.22) we obtain the error recursion

$$e^{n+1} = Re^n + \frac{\tau}{2}R_+^{-1}(y^n - \widetilde{y}^n) + \frac{\tau^2}{4}R_+^{-1}(z^n - \widetilde{z}^n) + \delta_{\mathrm{IMEX}}^{n+1},$$

cf. [91, (4.31)]. With

$$\triangle f^j = f^j - \widetilde{f}^j - f^{j+1} + \widetilde{f}^{j+1} \tag{4.26}$$

we have

$$y^n - \widetilde{y}^n = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \triangle f^j \qquad \text{and} \qquad z^n - \widetilde{z}^n = \begin{pmatrix} 1 \\ 0 \\ \frac{1}{\lambda} \end{pmatrix} \triangle f^j.$$

(2) *Stability.* For $e^0 = 0$ it holds that

$$e^n = \sum_{\ell=1}^{n} R^{n-\ell}\left(\frac{\tau}{2}R_+^{-1}(y^{\ell-1} - \widetilde{y}^{\ell-1}) + \frac{\tau^2}{4}R_+^{-1}(z^{\ell-1} - \widetilde{z}^{\ell-1}) + \delta_{\mathrm{IMEX}}^{\ell}\right).$$

Analogously to [91, (4.32)], taking the norm and using the triangle inequality, we obtain the estimate

$$\begin{aligned}\|e^n\|_X \leq \tau \sum_{\ell=1}^{n} \mathrm{e}^{(n-\ell)\tau c_m}\left(\frac{1}{2}\|y^{\ell-1} - \widetilde{y}^{\ell-1}\|_X + \frac{\tau}{4}\|R_+^{-1}(z^{\ell-1} - \widetilde{z}^{\ell-1})\|_X\right) \\ + \left\|\sum_{\ell=1}^{n} R^{n-\ell}\delta_{\mathrm{IMEX}}^{\ell}\right\|_X,\end{aligned} \tag{4.27}$$

Recalling the spaces from (4.2), we estimate similarly to [91, (4.33)]

$$\begin{aligned}\|y^\ell - \widetilde{y}^\ell\|_X = \|\triangle f^\ell\|_H &\leq L_\rho\big(\|u^\ell - \widetilde{u}^\ell\|_V + \|u^{\ell+1} - \widetilde{u}^{\ell+1}\|_V\big) \\ &\leq \frac{L_\rho}{\sqrt{\alpha}}\big(\|e^\ell\|_X + \|e^{\ell+1}\|_X\big).\end{aligned}$$

Therefore, we obtain

$$\begin{aligned}\frac{1}{2}\sum_{\ell=1}^{n} \mathrm{e}^{(n-\ell)\tau c_m}\|y^{\ell-1} - \widetilde{y}^{\ell-1}\|_X &\leq \sum_{\ell=1}^{n} \mathrm{e}^{(n-\ell)\tau c_m}\frac{L_\rho}{2\sqrt{\alpha}}\big(\|e^\ell\|_X + \|e^{\ell-1}\|_X\big) \\ &\leq \sum_{\ell=0}^{n} \frac{L_\rho}{\sqrt{\alpha}}\mathrm{e}^{(n-\ell)\tau c_m}\|e^\ell\|_X.\end{aligned}$$

From

$$R_+^{-1} z^n = \begin{pmatrix} 1 \\ \frac{\widetilde{\alpha}\tau}{2}\Delta_{\Omega,\Gamma} \\ \frac{1}{\lambda\gamma_+} \end{pmatrix} \otimes Q_+^{-1}(f^n - f^{n+1}),$$

and the notation (4.26) we obtain

$$\begin{aligned} &\frac{\tau}{4}\left\|R_+^{-1}(z^\ell - \widetilde{z}^\ell)\right\|_X \\ &\quad = \frac{1}{2}\left(\alpha\left\|\frac{\tau}{2}Q_+^{-1}\triangle f^\ell\right\|_V^2 + \left\|\frac{\tau^2}{4}\widetilde{\alpha}\Delta_{\Omega,\Gamma}Q_+^{-1}\triangle f^\ell\right\|_H^2 + \mu\left\|\frac{\tau}{2}\frac{1}{\lambda\gamma_+}Q_+^{-1}\triangle f^\ell\right\|_V^2\right)^{\frac{1}{2}} \end{aligned}$$

and from (4.21a) and (4.21b) we conclude

$$\begin{aligned} \alpha\left\|\frac{\tau}{2}Q_+^{-1}w\right\|_V^2 &\leq \frac{\alpha}{2\widetilde{\alpha}}\left\|w\right\|_H^2, \\ \mu\left\|\frac{\tau}{2}\frac{1}{\lambda\gamma_+}Q_+^{-1}w\right\|_V^2 &\leq \frac{\mu}{2(\lambda\gamma_+)^2\widetilde{\alpha}}\left\|w\right\|_H^2. \end{aligned}$$

This yields

$$\begin{aligned} &\sum_{\ell=1}^n \frac{\tau \mathrm{e}^{(n-\ell)\tau \mathrm{c}_m}}{4}\left\|R_+^{-1}(z^{\ell-1} - \widetilde{z}^{\ell-1})\right\|_X \\ &\qquad \leq \sum_{\ell=1}^n \frac{L_\rho \mathrm{e}^{(n-\ell)\tau \mathrm{c}_m}}{\sqrt{2\alpha}}\left(\left\|u^\ell - \widetilde{u}^\ell\right\|_{V_\alpha} + \left\|u^{\ell-1} - \widetilde{u}^{\ell-1}\right\|_{V_\alpha}\right) \\ &\qquad \leq \sum_{\ell=0}^n \frac{L_\rho\sqrt{2}}{\sqrt{\alpha}}\mathrm{e}^{(n-\ell)\tau \mathrm{c}_m}\left\|e^\ell\right\|_X. \end{aligned}$$

Inserting these bounds yields

$$\left\|e^n\right\|_X \leq \frac{\tau L_\rho}{\sqrt{\alpha}}(1+\sqrt{2})\sum_{\ell=0}^n \mathrm{e}^{(n-\ell)\tau \mathrm{c}_m}\left\|e^\ell\right\|_H + \left\|\sum_{\ell=1}^n R^{n-\ell}\delta_{\mathrm{IMEX}}^\ell\right\|_X.$$

(3) *Bound of defects from* (4.25). Since we already know that the Crank-Nicolson defect is bounded by $C\tau^3$, it remains to bound $\widetilde{\delta}^{\ell+1}$. We follow [91, p. 41] and split it into two parts

$$\widetilde{\delta}^{\ell+1} = \widetilde{\delta}_1^{\ell+1} + \widetilde{\delta}_2^{\ell+1}$$

with

$$\widetilde{\delta}_1^{\ell+1} = \frac{\tau}{4}\begin{pmatrix} \tau Q_+^{-1} \\ Q_- Q_+^{-1} \\ \frac{\tau}{\lambda\gamma_+}Q_+^{-1} \end{pmatrix} \otimes (\widetilde{f}^\ell - \widetilde{f}^{\ell+1}), \qquad \widetilde{\delta}_2^{\ell+1} = \frac{\tau}{4}\begin{pmatrix} 0 \\ -(\widetilde{f}^\ell - \widetilde{f}^{\ell+1}) \\ 0 \end{pmatrix},$$

and then combine terms from two different steps to gain an extra order of τ. We observe that

$$\widetilde{\delta}_1^{\ell+1} + R\widetilde{\delta}_2^\ell = \frac{\tau}{2}\begin{pmatrix} \frac{\tau}{2}Q_+^{-1} \\ \frac{1}{2}Q_- Q_+^{-1} \\ \frac{\tau}{2\lambda\gamma_+}Q_+^{-1} \end{pmatrix} \otimes (-\widetilde{f}^{\ell-1} + 2\widetilde{f}^\ell - \widetilde{f}^{\ell+1}). \tag{4.28}$$

For the difference quotients we have the bounds

$$\left\|\widetilde{\delta}_2^{\ell+1}\right\|_X = \frac{\tau}{4}\left\|\widetilde{f}^{\ell} - \widetilde{f}^{\ell+1}\right\|_H \leq C\tau^2, \qquad \tau\left\|\widetilde{f}^{\ell-1} - 2\widetilde{f}^{\ell} + \widetilde{f}^{\ell+1}\right\|_H \leq C\tau^3. \tag{4.29}$$

To be more precise, we denote by $\mathcal{I}^\ell = [t_{\ell-1}, t_{\ell+1}]$ and as in [91, (4.36)] we obtain, due to the regularity assumptions on u, that

$$\begin{aligned}\tau\left\|\widetilde{f}^{\ell-1} - 2\widetilde{f}^{\ell} + \widetilde{f}^{\ell+1}\right\|_H &\leq C\tau^3 \left\|\partial_t^2\big(u'' - \Delta_{\Omega,\Gamma}(\alpha u - \beta^T M)\big)\right\|_{L^\infty(\mathcal{I}^\ell,H)} \\ &\leq C\tau^3\left(\left\|u^{(4)}\right\|_{L^\infty(\mathcal{I}^\ell,H)} + \left\|\partial_t^2\big(\alpha u + \beta^T M\big)\right\|_{L^\infty(\mathcal{I}^\ell,H^2)}\right).\end{aligned}$$

where $H^2 = H^2(\Omega)$ for (D) and $H^2 = H^2(\Omega,\Gamma)$ in the case (K). Using the same arguments, we find that defects $\widetilde{\delta}_1^1$, $\widetilde{\delta}_2^n$ are of order τ^2. Therefore, we estimate

$$\begin{aligned}\tau\left\|\widetilde{f}^{\ell} - \widetilde{f}^{\ell+1}\right\|_H &\leq C\tau^2 \left\|\partial_t\big(u'' - \Delta_{\Omega,\Gamma}(\alpha u - \beta^T M)\big)\right\|_{L^\infty(\mathcal{I}^\ell,H)} \\ &\leq C'\tau^2\left(\left\|u^{(3)}\right\|_{L^\infty(\mathcal{I}^\ell,H)} + \left\|\partial_t\big(\alpha u + \beta^T M\big)\right\|_{L^\infty(\mathcal{I}^\ell,H^2)}\right).\end{aligned}$$

Then, using (4.25) we split

$$\left\|\sum_{\ell=1}^n R^{n-\ell}\delta_{\mathrm{IMEX}}^\ell\right\|_X \leq \left\|\sum_{\ell=1}^n R^{n-\ell}\delta_{\mathrm{CN}}^\ell\right\|_X + \left\|\sum_{\ell=1}^n R^{n-\ell}(\widetilde{\delta}_1^\ell + \widetilde{\delta}_2^\ell)\right\|_X$$

and with an index shift and the previous calculations, we see

$$\begin{aligned}\left\|\sum_{\ell=1}^n R^{n-\ell}(\widetilde{\delta}_1^\ell + \widetilde{\delta}_2^\ell)\right\|_X &= \left\|\sum_{\ell=1}^n R^{n-\ell}\widetilde{\delta}_1^\ell + R^{n-\ell-1}R\widetilde{\delta}_2^\ell\right\|_X \\ &= \left\|R^{n-1}\widetilde{\delta}_1^1 + \widetilde{\delta}_1^n + \sum_{\ell=2}^n R^{n-\ell}(\widetilde{\delta}_1^\ell + R\widetilde{\delta}_2^\ell)\right\|_X \\ &\leq \mathrm{e}^{n\tau\mathrm{c}_m}\left(\left\|\widetilde{\delta}_1^1\right\|_X + \left\|\widetilde{\delta}_2^n\right\|_X + \sum_{\ell=2}^n\left\|\widetilde{\delta}_1^\ell + R\widetilde{\delta}_2^\ell\right\|_X\right) \\ &\leq C\mathrm{e}^{T\mathrm{c}_m}\tau^2.\end{aligned}$$

In the last estimate we used $t_n \leq T$, (4.28), (4.29), and that $\left\|\tau Q_+^{-1}\right\|_{V\leftarrow H} \leq C$ and $\left\|Q_- Q_+^{-1}\right\|_{H\leftarrow H} \leq C$ by Lemma 4.5.

With the stability bound (4.27), we see

$$\begin{aligned}\mathrm{e}^{-t_n\mathrm{c}_m}\left\|e^n\right\|_X &\leq \frac{\tau L_\rho}{\sqrt{\alpha}}(1+\sqrt{2})\sum_{\ell=0}^n \mathrm{e}^{-\ell\tau\mathrm{c}_m}\left\|e^\ell\right\|_X + \mathrm{e}^{-t_n\mathrm{c}_m}\left\|\sum_{\ell=1}^n R^{n-\ell}\delta_{\mathrm{IMEX}}^\ell\right\|_X \\ &\leq \frac{\tau L_\rho}{\sqrt{\alpha}}(1+\sqrt{2})\sum_{\ell=0}^n \mathrm{e}^{-\ell\tau\mathrm{c}_m}\left\|e^\ell\right\|_X + C\tau^2.\end{aligned}$$

Finally, the desired error bound follows from applying Grönwall's Lemma provided that x^n is uniformly bounded in X. The latter follows along the lines of [90, Thm. 4.9]. □

Remark 4.9. The full discretization can be done analogously to [77] with isoparametric finite elements, see also [46]. Using the time discretization error analysis from the previous section, the full error estimate is a combination thereof with the one shown in [77]. When it comes to lift and reference operators for the error of space discretization, the additional variables M_j are treated in the same manner as u.

4.4 Numerical experiments

In this section we show numerical examples to support our theoretical results. We consider the wave equation (4.1) with kinetic boundary conditions on the unit disc $B(0,1) \subset \mathbb{R}^2$. In order to measure exact numerical errors, we extend an example from [77] by including a convolution with $m = 4$ and the parameters $\alpha = 1, \beta_1 = 1, \beta_2 = 1.5, \beta_3 = 2, \beta_4 = 1.25$ and $\lambda_1 = 0.2, \lambda_2 = 1, \lambda_3 = 1.5, \lambda_4 = 2$. We choose the nonlinearities

$$\begin{aligned} f_\Omega(t,\xi,u) &= |u|\,u + \eta_\Omega(t,\xi), \\ f_\Gamma(t,\xi,u) &= |u|^2\,u + \eta_\Gamma(t,\xi), \end{aligned}$$

where

$$\begin{aligned} \eta_\Omega(t,\xi) &= -\big(4\pi^2 + |\sin(2\pi t)\xi_1\xi_2|\big)\sin(2\pi t)\xi_1\xi_2, \\ \eta_\Gamma(t,\xi) &= (6c^2 - 4\pi^2)\xi_1\xi_2\sin(2\pi t) - \big(\sin(2\pi t)\xi_1\xi_2\big)^3 \\ &\quad - 12\pi\sum_{j=1}^{m}\frac{\beta_j}{4\pi^2+\lambda_j}\big(\mathrm{e}{-\lambda_j t} - \cos(2\pi t) + \frac{\lambda_j}{2\pi}\sin(2\pi t)\big). \end{aligned}$$

The initial values are set to be

$$u(0,\xi) = 0, \qquad \partial_t u(0,\xi) = 2\pi\xi_1\xi_2,$$

and the exact solution to this example is given by

$$u(t,\xi) = \sin(2\pi t)\xi_1\xi_2.$$

The codes to reproduce our results are available at

`https://github.com/MalikScheifinger/WaveKineticBC.git`

The space discretization software is based on the FEM library `deal.II` [8] version 9.5.0, using quadrilateral mesh elements and isoparametric finite elements with polynomial degree $p = 2$ and maximal mesh width $h_{\max} \approx 0.014$. Our implementation follows [91, Chapter 6.2]. We shortly specify the notation we use and state our in space discretized IMEX scheme. We denote by $\boldsymbol{\mathcal{M}} \in \mathbb{R}^{N\times N}$ the mass matrix, by $\boldsymbol{\mathcal{S}} \in \mathbb{R}^{N\times N}$ the stiffness matrix and the load vector by $\boldsymbol{f}^n$ after choosing the standard nodal basis. Then the scheme reads

$$\begin{aligned} \boldsymbol{\mathcal{M}}\boldsymbol{v}^{n+\frac{1}{2}} &= \boldsymbol{\mathcal{M}}\boldsymbol{v}^n - \frac{\tau}{2}\boldsymbol{\mathcal{S}}(\alpha\boldsymbol{u}^n + \widetilde{\beta}^T\boldsymbol{M}^n) - \frac{\tau^2}{4}\widetilde{\alpha}\boldsymbol{\mathcal{S}}\boldsymbol{v}^{n+\frac{1}{2}} + \frac{\tau}{2}\boldsymbol{f}^n, \qquad (4.30a) \\ \boldsymbol{u}^{n+1} &= \boldsymbol{u}^n + \tau\boldsymbol{v}^{n+\frac{1}{2}}, \\ \boldsymbol{M}_j^{n+1} &= \gamma_j\boldsymbol{M}_j^n + \gamma_{j,+}^{-1}\frac{\tau}{\lambda_j}\boldsymbol{v}^{n+\frac{1}{2}}, \\ \boldsymbol{\mathcal{M}}\boldsymbol{v}^{n+1} &= -\boldsymbol{\mathcal{M}}\boldsymbol{v}^n + 2\boldsymbol{\mathcal{M}}\boldsymbol{v}^{n+\frac{1}{2}} + \frac{\tau}{2}(\boldsymbol{f}^{n+1} - \boldsymbol{f}^n). \end{aligned}$$

The linear system (4.30a) is equivalent to

$$\boldsymbol{\mathcal{Q}}_+\boldsymbol{v}^{n+\frac{1}{2}} = \boldsymbol{\mathcal{M}}\boldsymbol{v}^n - \frac{\tau}{2}\boldsymbol{\mathcal{S}}(\alpha\boldsymbol{u}^n + \widetilde{\beta}^T\boldsymbol{M}^n) + \frac{\tau}{2}\boldsymbol{f}^n, \qquad \boldsymbol{\mathcal{Q}}_+ = \boldsymbol{\mathcal{M}} + \frac{\tau^2}{4}\widetilde{\alpha}\boldsymbol{\mathcal{S}}.$$

We solve this linear system with the conjugate gradient method and SSOR preconditioning.

In Figure 4.1 we show the numerical approximation of (4.1) using the data given in Section 4.4 at four different times.

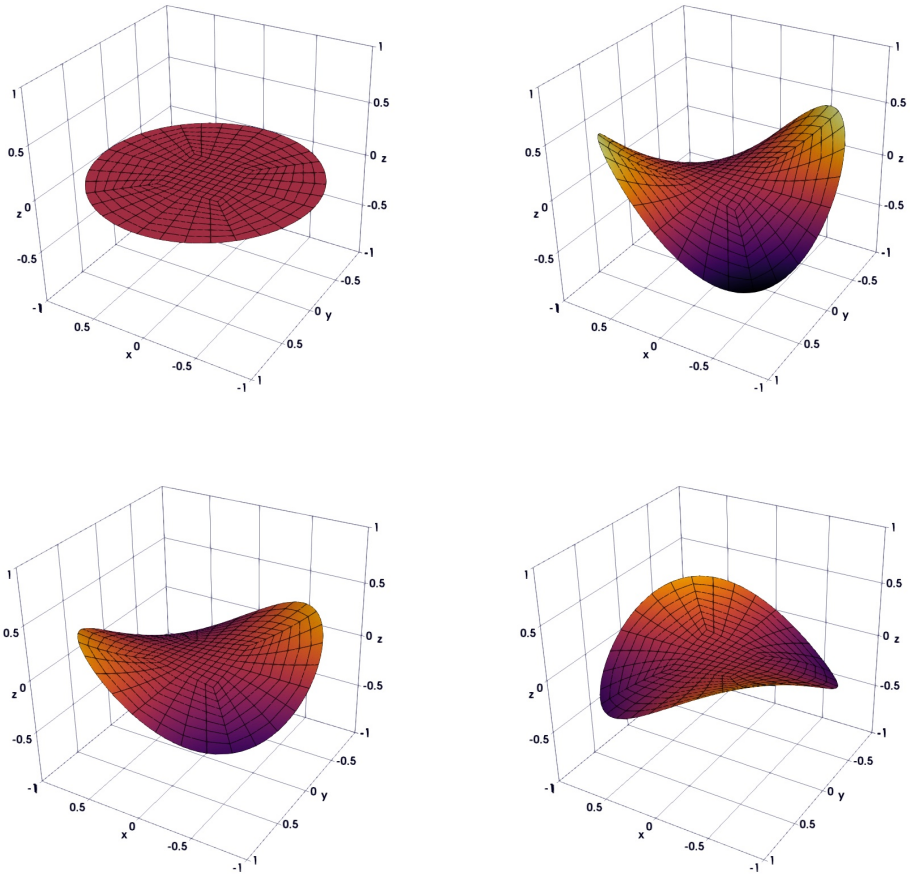

Figure 4.1: Snapshots of the solution at times $t = 0, 0.2, 0.4, 0.6$ (from top left to bottom right) using the IMEX method with time stepsize $\tau = 0.1$.

In Figure 4.2 we illustrate the error of our method against the time stepsize τ. The error is measured at the endtime $T = 0.8$ in the $V_\alpha \times H$ norm. We observe second-order convergence in time.

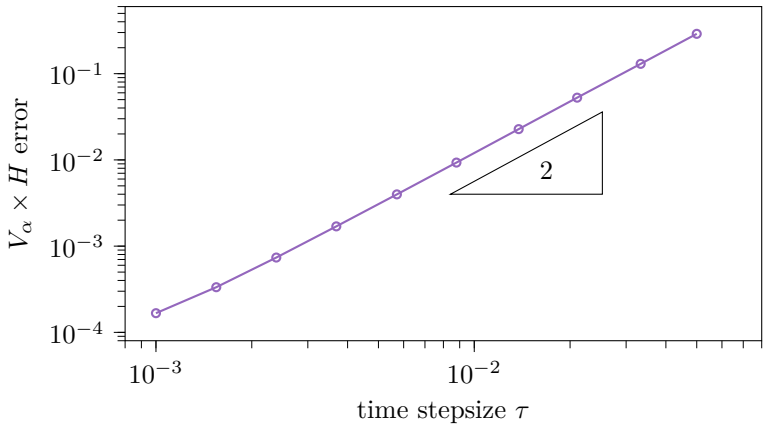

Figure 4.2: Error evaluated at the endtime $T = 0.8$ in the $V_\alpha \times H$ norm plotted against time stepsize τ.

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