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Nonlinear Optics: Physics, Analysis, and Numerics

Organized by
Kurt Busch, Berlin
Ramy El-Ganainy, Houghton
Marlis Hochbruck, Karlsruhe

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Abstract. When high-intensity electromagnetic waves at optical frequencies interact with solids and/or nanostructures the materials' response cannot anymore be described via simple linear relations. The resulting science of nonlinear optics has recently witnessed exiting developments that have brought to the fore numerous mathematical challenges that need to be addressed in order to fully exploit the opportunities that result from these developments. The mathematical modeling involves a system of partial differential equations where the Maxwell equations are coupled to evolution equations of the materials and their response to electromagnetic fields. Typically, the full coupled systems are quite complicated or even intractable so that the derivation, the analysis, and the numerical treatment of simplified effective models is often indispensable. In turn, this requires the close cooperation between researchers from theoretical physics and analysis/numerics in order to push forward the field on nonlinear optics.

Mathematics Subject Classification (2020): 35-XX, 65-XX, 78-XX.

Introduction by the Organizers

Nonlinear optics is concerned with the interaction of high-intensity light waves with material bodies. While light propagation is described via the Maxwell equations, the adequate description of the material response proceeds via different types of evolution equations such as rate equations, Bloch equations or the (single- or many-particle) Schrödinger equations and material interfaces require the formulation of corresponding boundary conditions.

The numerical approximation of the resulting coupled systems of partial differential equations is challenging because the light source may operate in continuous-wave mode or may deliver pulses with durations that can range from nano- via pico- all the way to femto- and, nowadays, even tens of attoseconds. New advances in the numerics of highly oscillatory problems, which also work in settings of low regularity, are very promising here. Similarly, the materials' relevant length and and/or time scales may vary over many orders of magnitude. This requires homogenization and multiscale of localized orthogonal decomposition methods.

Conversely, in case of very dissimilar scales, one may "integrate out" (eliminate) the fast scale(s) in one sub-system, leading to effective nonlinear evolution equations for the other sub-system. Classic examples are different types of nonlinear Schrödinger equations in various settings such as fiber optics or cold-atom optics as well as wave equations with second- and/or third-order nonlinearities. Clearly, this "integrating out" has to be exercised in a mathematically consistent fashion so that symmetries, conservation laws etc. of the underlying coupled systems are preserved. In addition, theoretical tools have to be developed that facilitate the analysis of the effective equations' solution structure and similar statements apply to the effective equations' numerical treated.

The above-sketched scenario presents the mathematical and theoretical-physics background of nonlinear optics against which the significant experimental progress, notably in the development of novel laser sources and advances in material growth and nanostructuring, has to be viewed. Clearly, the full exploitation of this potential of nonlinear optics requires the continuous advancement of a comprehensive analytical framework and innovative numerical methods. Specifically, this requires the close cooperation of researchers from theoretical physics and mathematics in order to develop physically meaningful material models that are mathematically well-posed and consistent. Wellposedness and consistency are essential to analyze the structure of the solution and to construct efficient numerical schemes.

The purpose of the workshop "Nonlinear optics: physics, analysis and numerics" has been to facilitate the exchange of ideas and discussions of future directions of researchers who work in the interdisciplinary field of nonlinear optics that lies at the intersection of applied mathematics and theoretical physics. The workshop started with several kick-off presentation of a number of mathematical challenges that physicists are facing in their work. From there on, numerous lively discussions between different groups of mathematicians and physicists emerged and, following the progress of these discussions, the organizers coordinated a balanced sequence of longer presentations by the participants. On the one hand, these presentations provided additional stimuli such as providing up-to-date summaries and results of certain mathematical techniques and the current state of material models. On the other hand, these presentations opened new fields for exchanging ideas. The latter is very well illustrated via the topic of spectral theory for non-Hermitian systems. After the importance of light wave transport and localization in disordered non-Hermitian photonic systems was introduced, there followed an impromptu-presentation on the spectral theory of non-Hermitian matrices and several exciting

follow-up discussions. Similarly, the former is well illustrated by the presentation of the state-of-the-art in large-scale computations of coupled Maxwell-Schrödinger systems which led to several stimulating follow-up presentations and discussions on the construction and use of multi-step integration methods. Over the course of the workshop, several other discussion lines were followed. Besides the plenary presentations, the organizers provided ample time for meetings in small groups, so that specific topics could be studied in much more detail.

Overall, the workshop has greatly benefited from both, active contributions by all workshop participants, junior and senior researchers alike, and the immensely inspiring atmosphere provided by the MFO facilities and the MFO staff members. In fact, it is the organizers' considered opinion that bringing together theoretical physicists and mathematicians has started a number of promising discussions that have significant potential for fruitful and productive collaborations that reach well beyond the workshop.

Workshop: Nonlinear Optics: Physics, Analysis, and Numerics

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Abstracts

Computing certain invariants of topological spaces of dimension three

Heiko Appel

This presentation is introducing the theoretical foundations and the implementation details of a density-functional approach for coupled photons, electrons, and effective nuclei in non-relativistic quantum electrodynamics that we have developed over the past years in our group at the Max Planck Institute for the Structure and Dynamics of Matter in Hamburg (Advances in Physics, 2019 Vol. 68, No. 4, 225–333). Starting point of the formalism is a generalization of the Pauli–Fierz field theory for which we establish a one-to-one correspondence between external fields and internal variables. Based on this correspondence, we introduce a Kohn-Sham construction which provides a computationally feasible approach for ab-initio light-matter interactions. In the mean-field limit, the formalism reduces to coupled Ehrenfest–Maxwell–Pauli–Kohn–Sham equations. Within this formalism, we show how to couple the time-evolution of the electromagnetic fields self-consistently with the quantum time-evolution of the electrons and nuclei. We present an implementation of the approach in the real-space real-time code Octopus (https://octopus-code.org) using the Riemann–Silberstein formulation of classical electrodynamics to rewrite Maxwell's equations in Schrödinger form. Furthermore, adapting established multi-trajectory methods that have been developed for electron-nuclear problems to coupled electron-photon systems, we show how to recover quantum effects such as spontaneous emission in real-time from ensembles of Maxwell-Kohn-Sham trajectories.

Hierarchies of integrable NLS-type equations and selected solutions

Uwe Bandelow

Infinite hierarchies of integrable Nonlinear Schrödinger (NLS)-type evolution equations are presented. The 2nd order member of these hierarchies is the NLS. From the 3rd order on, these hierarchies branch. The Hirota-branch is based on Lax-pairs in terms of 2x2 matrices, and contains the Hirota Equation in 3rd order, the Lakshmanan-Porsezian-Daniels (LPD) Equation in 4th order, and can be extended by infinite many independent terms of higher order. With increasing order, these terms become increasingly complicated, but all of them provide integrable contributions. The construction of this hierarchy allows to pursue special known analytic solutions, such as solitons, breathers, and rogue waves throughout this hierarchy [1].

Another hierarchy branches in 3rd order from the NLS with the Sasa-Satsuma Equation (SSE) [2, 3], which is based on Lax-pairs in terms of 3x3 matrices. It contains another 4th order contribution, which is new and different from the LPD equation. Also this (SSE-)hierarchy can be extended by infinite many independent higher-order terms, which again become increasingly complicated, but all of

them are integrable contributions. Also here, special solutions such as solitons, breathers, and rational solutions of SSE are known [4, 5, 6], but still have to be explored throughout the hierarchy. A very general breather solution family (with 7 family parameters) to the SSE is shown to contain almost all known soliton solutions as special limits [4, 6], if taken with care, and in particular rational solutions [5], known as rogue waves.

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Improved uniform error bounds of the time-splitting methods for the long-time (nonlinear) Schrödinger equation and applications

Weizhu Bao

The (nonlinear) Schrödinger equation arises in various physical phenomena, such as quantum mechanics, Bose–Einstein condensates, laser beam propagation, plasma and particle physics. In this talk, we consider the following Schrödinger equation

$$i\partial_t \psi(\mathbf{x},t) = -\Delta\psi(\mathbf{x},t) + \varepsilon V(\mathbf{x})\psi(\mathbf{x},t),\ \mathbf{x}\in\Omega,\ t>0, \tag{1}$$

and the nonlinear Schrödinger equation (NLSE)

$$i\partial_t \psi(\mathbf{x},t) = -\Delta\psi(\mathbf{x},t) \pm \varepsilon^2|\psi(\mathbf{x},t)|^2\psi(\mathbf{x},t),\ \mathbf{x}\in\Omega,\ t>0, \tag{2}$$

with the initial data $\psi(\mathbf{x},0)=\psi_0(\mathbf{x})$ for $\mathbf{x}\in\overline{\Omega}$, where $\Omega=\prod_{i=1}^d(a_i,b_i)\subset\mathbb{R}^d$ $(d=1,2,3)$ is a bounded domain equipped with periodic boundary conditions. Here, t is time, $\mathbf{x}=(x_1,\cdots,x_d)^T\in\mathbb{R}^d$ is the spatial coordinate, $\psi(\mathbf{x},t)\in\mathbb{C}$ is the complex order parameter/wave function, $V(\mathbf{x})\in\mathbb{R}$ is a given external potential, $\varepsilon\in(0,1]$ is a dimensionless parameter.

The Schrödinger equation (1) and the nonlinear Schrödinger equation (2) are discretized numerically by the time-splitting Fourier pseudospectral (TSFP) method [1]. Let h be the mesh size, τ be the time step size, $t_n=n\tau$ for $n\geq 0$, and $T>0$ be a fixed time. By adopting the technique of *regularity compensation oscillation* (RCO) in which the high frequency modes are controlled by regularity and the low frequency modes are analyzed by phase cancellation and energy method, we established the following improved uniform error bounds on the TSFP method as following: [1]:

Theorem 1. *Let ψ^n be the numerical approximation of the Schrödinger equation* (1) *obtained from the TSFP method. Under proper assumptions on the exact solution $\psi := \psi(\mathbf{x}, t)$ and the potential $V(\mathbf{x})$* [1]*, for any $0 < \varepsilon \leq 1$, we have* [1]

$$\|\psi(x, t_n) - I_N \psi^n\|_{L^2} \leq (C_0 + C_1 \varepsilon t_n) \tilde{C}(T) \left(h^m + \tau^2\right), \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau}, \tag{3}$$

where $m \geq 2$, I_N is the standard trigonometric interpolation operator, C_0 and C_1 are two positive constants independent of h, τ, n, ε and T, $\tilde{C}(T)$ depends on $\|\psi\|_{L^\infty([0,T];H^m)}$ and $\|V\|_{H^{m^*}}$ with $m^* = \max\{m, 5\}$.

Theorem 2. *Let ψ^n be the numerical approximation of the Schrödinger equation* (1) *obtained from the TSFP method. Under proper assumptions on the exact solution $\psi := \psi(\mathbf{x}, t)$ and the potential $V(\mathbf{x})$* [1]*, for any $\varepsilon \in (0, 1]$ and a fixed $\tau_0 \in (0, 1)$, under some conditions on τ* [1]*, we have the estimates*

$$\|\psi(x, t_n) - I_N \psi^n\|_{H^1} \lesssim h^{m-1} + \varepsilon \tau^2 + \tau_0^{m-1}, \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau}. \tag{4}$$

where $m \geq 3$. In particular, if the exact solution is smooth, i.e. $\psi(x, t) \in H^\infty_{\rm per}$, the τ_0^{m-1} part error would decrease exponentially in terms of τ_0 and can be ignored in practical computation when τ_0 is taken as $\tau_0^{\rm cr}$ (small but fixed, only depends on ψ and the logarithm of the machine precision), thus the improved error bounds for sufficiently small τ could be stated as [1]

$$\|\psi(x, t_n) - I_N \psi^n\|_{H^1} \lesssim h^{m-1} + \varepsilon \tau^2, \quad 0 \leq n \leq \frac{T/\varepsilon}{\tau}. \tag{5}$$

Theorem 3. *Let ψ^n be the numerical approximation of the nonlinear Schrödinger equation* (2) *obtained from the TSFP method* [1]*. Under proper assumptions on the exact solution $\psi := \psi(\mathbf{x}, t)$* [1]*, there exist $h_0 > 0$, $0 < \tau_0 < 1$ sufficiently small and independent of ε such that, for any $0 < \varepsilon \leq 1$, when $0 < h < h_0$ and some conditions on τ* [1]*, the following error bounds hold* [1]

(6)

$$\|\psi(x, t_n) - I_N \psi^n\|_{H^1} \lesssim h^{m-1} + \varepsilon^2 \tau^2 + \tau_0^{m-1}, \quad \|I_N \psi^n\|_{H^1} \leq 1 + M, \ 0 \leq n \leq \frac{T/\varepsilon^2}{\tau},$$

where $m \geq 5$, $M := \|\psi\|_{L^\infty([0,T_\varepsilon];H^1)}$ with $T_\varepsilon = \frac{T}{\varepsilon^2}$. In particular, if the exact solution is smooth, i.e. $\psi(x, t) \in H^\infty_{\rm per}$, the τ_0^{m-1} error part would decrease exponentially and can be ignored in practical computation when τ_0 is small but fixed, and thus the estimate would practically become

$$\|\psi(x, t_n) - I_N \psi^n\|_{H^1} \lesssim h^{m-1} + \varepsilon^2 \tau^2. \tag{7}$$

Similar error bounds can be established on the time-splitting methods for the long-time dynamics of the Dirac equation with small electromagnetic potential [2], for the long-time dynamics of the nonlinear Dirac equation with weak cubic nonlinearity [3], and for the long-time dynamics of the nonlinear Klein-Gordon equation with weak cubic nonlinearity [4, 5, 6].

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Numerical approximation of nonlinear Schrödinger equations: classical vs. modern methods

Christian Döding

We consider the nonlinear Schrödinger equation (NLS) of the form

$$\mathrm{i}\partial_t u = -\Delta u + Vu + \beta|u|^2 u \quad \text{in } \Omega \times [0,T] \tag{1}$$

on a convex, bounded, and polyhedral domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$ with homogeneous Dirichlet boundary conditions and on a time interval $[0, T]$ with a sufficiently smooth initial value u_0. The function $V \in L^\infty(\Omega, \mathbb{R}_{\geq 0})$ is a positive and bounded external potential and $\beta \in \mathbb{R}$ plays the role of an interaction parameter. The NLS has wide applications in modern physics and especially in nonlinear optics as a model for light propagation in complex media such as glass fiber, see [6] for more details.

Numerical approximations of (1) have been studied extensively in the last decades, including classical approaches such as finite element methods and spectral methods for spatial discretization together with structure preserving time integrators as well as splitting methods, see e.g. [2] and the references therein. In this contribution we propose and discuss a modern approach from [2] based on spatial discretization by localized orthogonal decomposition (LOD). The LOD is a multiscale approach which was first introduced in [5] in the context of elliptic multiscale problems and which turned out to be very suitable also for the NLS as shown in [1, 2, 3]. We combine the space discretization with a energy preserving time integrator of high order which was first posed for the NLS in combination with standard finite elements in space in [4]. We briefly recapitulate the derivation of the method from [2] and discuss its properties and possible future developments.

1. Space-Time Discretization

For the space discretization we start with a suitable triangulation $\mathcal{T}_h$ of the domain Ω into triangles of size $h > 0$. A classical Lagrange finite element discretization of order one is based on the approximation space $V_h := \{v \in C(\overline{\Omega}) \cap H_0^1(\Omega) : v_{|K} \in \mathbb{P}_1(K),\ K \in \mathcal{T}_h\}$, i.e. the space of continuous and piecewise linear functions in $H_0^1(\Omega)$. The L^2-projection $P_h : L^2(\Omega) \to V_h$ onto the finite element space has a kernel $W_h := \{v \in L^2(\Omega) : P_h v = 0\}$ which, roughly speaking, consists of functions containing details that the approximation space V_h cannot resolve. In particular, the stable decomposition $H_0^1(\Omega) = V_h \oplus W_h$ with orthogonality $V_h \perp_{(\cdot,\cdot)} W_h$ holds with respect to the L^2 scalar product $(v, w) = \int_\Omega v\,\overline{w}\,dx$. The idea of the LOD is to define a new approximation space V_{LOD}, which incorporates information of (1) via the sesquilinear form

$$a(v, w) := (\nabla v, \nabla w) + (Vv, w).$$

Precisely, we choose V_{LOD} to be the $a(\cdot,\cdot)$-orthogonal complement of W_h, i.e., $V_{\mathrm{LOD}} \perp_{a(\cdot,\cdot)} W_h$ and the orthogonal decomposition $H_0^1(\Omega) = V_{\mathrm{LOD}} \oplus W_h$ holds. This space satisfies $\dim V_{\mathrm{LOD}} = \dim V_h$ and has very nice approximation properties as elaborated in [2, 3] and in the references therein.

For the time discretization we choose an energy preserving continuous Galerkin time integrator from [4] and combine it with the LOD in space as proposed in [2]. We start by partitioning the time interval into time instances $t_n = n\tau$, $n = 0, \dots, N \in \mathbb{N}$ with a step size $\tau = T/N > 0$. For a polynomial degree $q \in \mathbb{N}$, we define the test space

$$\tilde{W}_{\mathrm{LOD}}^q := \{v : [0, T] \to V_{\mathrm{LOD}} : v_{|(t_n, t_{n+1}]} = \sum_{j=0}^{q} t^j \phi_{n,j},\ \phi_{n,j} \in V_{\mathrm{LOD}}\}$$

and ansatz space $W_{\mathrm{LOD}}^q := \tilde{W}_{\mathrm{LOD}}^q \cap C([0, T], V_{\mathrm{LOD}})$, so that our fully-discrete scheme (in a slightly simplified version, cf. [2]) can be formulated in the sense of a space-time method: Find $\tilde{u} \in W_{\mathrm{LOD}}^q$ such that $\tilde{u}(t_0) = P_{\mathrm{LOD}}(u_0)$ and

$$\int_0^T (\mathrm{i}\partial_t \tilde{u}, v) - (\nabla \tilde{u}, \nabla v) - (V\tilde{u}, v) - \beta(|\tilde{u}|^2 \tilde{u}, v)\,dt = 0 \quad \forall v \in \tilde{W}_{\mathrm{LOD}}^{q-1} \tag{2}$$

where P_{LOD} is a suitable projection onto V_{LOD}. We refer to [2, 3] and the references therein for more details on the LOD and the implementation of the method.

2. Discussion

As it was shown numerically in [1, 2] the scheme (2) is expected to be convergent of order $h^3 + \tau^{2q}$ under relatively mild regularity assumptions on the solution u. In particular, for rough potentials $V \in L^\infty(\Omega)$ without any further regularity, this order of convergence has been verified numerically in [1], although the solution is not H^4-regular. A classical finite element approximation of order three has the same order of convergence for smooth problems but cannot compete in the case of rough potentials due to the lack of regularity. Similar observations are made in [3] where the spatial LOD discretization is compared to a spectral method in the

case of rough potentials. Furthermore, as shown in [3], the LOD approximation in space is an order six approximation of the energy of the system (1), which is another important feature for solving the NLS. Further improvements of the method, a rigorous error analysis, and possible applications to physics, especially to nonlinear optics, are left for future research.

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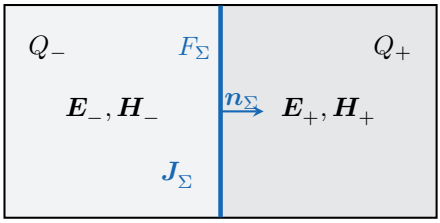
Numerical methods for nonlinear optics in plasmonic nanogaps

Benjamin Dörich, Julian Dörner

(joint work with Marlis Hochbruck)

We report on recent advances for the numerical discretization of linear Maxwell equations with inhomogeneous interface conditions. They appear for examples in experiments to investigate optical properties of thin material layers, such as Graphene or Transition Metal Dichalcogenides (TMDCs). We propose a discontinuous Galerkin discretization in space which weakly incorporates the jump condition, and apply a second-order time integration method to the spatially discrete equation.



We consider Maxwells equation on the cuboid $Q = Q_- \cup Q_+$, composed of the subcuboids $Q_- = (-1, 0) \times (0, 1)^2$ and $Q_+ = (0, 1) \times (0, 1)^2$, given by

$$\partial_t \boldsymbol{H}_\pm = -\mu_\pm^{-1} \operatorname{curl} \boldsymbol{E}_\pm, \qquad \text{in } [0, T] \times Q_\pm, \tag{1a}$$

$$\partial_t \boldsymbol{E}_\pm = \varepsilon_\pm^{-1} \operatorname{curl} \boldsymbol{H}_\pm, \qquad \text{in } [0, T] \times Q_\pm, \tag{1b}$$

with positive and bounded material parameters $\mu_\pm, \varepsilon_\pm$ and perfectly conducting boundary conditions $\boldsymbol{E} \times \boldsymbol{\nu} = 0$ on $[0,T] \times \partial Q$. On the interface F_Σ there hold the conditions

$$[\![\boldsymbol{H} \times \boldsymbol{n}_\Sigma]\!]_{F_\Sigma} = \boldsymbol{J}_\Sigma, \quad [\![\boldsymbol{E} \times \boldsymbol{n}_\Sigma]\!]_{F_\Sigma} = 0, \quad \text{on } [0,T] \times F_\Sigma,$$

where $[\![f]\!]_{F_\Sigma} = f_+\big|_{F_\Sigma} - f_-\big|_{F_\Sigma}$ denotes the jump and $\boldsymbol{J}_\Sigma$ is an external surface current. In the wellposedness analysis presented in [1], a lift operator $\mathcal{L} : L^2(F_\Sigma)^3 \to L^2(Q)^3$ is constructed which in particular satisfies

$$[\![(\boldsymbol{H} - \mathcal{L}\boldsymbol{J}_\Sigma) \times \boldsymbol{n}_\Sigma]\!]_{F_\Sigma} = 0.$$

Thus, we can consider the shifted variables $\big(\boldsymbol{H} - \mathcal{L}\boldsymbol{J}_\Sigma, \boldsymbol{E}\big)$ which lie in the standard state space $H(\operatorname{curl}, Q) \times H_0(\operatorname{curl}, Q)$. This allows us to apply semigroup theory to the shifted problem, and to obtain existence and stability of solutions.

For the discretization in space presented in [2], we discretize Q with a suitable mesh $\mathcal{T}_h$, which is aligned to the interface F_Σ. We then use an approximation space consisting of ansatz functions which are piecewise polynomials on each cell and denote this space by $\mathbb{P}_3^k(\mathcal{T}_h) = \big\{\, p \in L^2(Q) \;\big|\; p|_K \in \mathbb{P}_3^k(K) \,\big\}$, see for example [3]. Here, the mesh parameter h denotes the largest diameter of all cells and tends to zero for finer discretization. With this, we obtain the spatially discrete system

$$\partial_t \boldsymbol{H}_h(t) = -\operatorname{curl}_{0,h} \boldsymbol{E}_h(t), \tag{2a}$$

$$\partial_t \boldsymbol{E}_h(t) = \operatorname{curl}_h \boldsymbol{H}_h(t) - \mathcal{L}_h \boldsymbol{J}_\Sigma(t), \tag{2b}$$

where we denoted by curl_h the discrete curl operator, by curl_h the discrete curl operator which incorporates the homogeneous boundary condition of the electrical field, and $\mathcal{L}_h : L^2(F_\Sigma)^3 \to V_h$ is a discrete lift operator. We note that the support of $\mathcal{L}_h \boldsymbol{J}_\Sigma$ is only contained in the cells which touch the interface.

If we assume that the solution $\big(\boldsymbol{H}, \boldsymbol{E}\big)$ of (1) admits piecewise Sobolev regularity of order $k+1$ in space, we obtain for $t \in [0,T]$ convergence in the mesh-size of order k, i.e.,

$$\big\| \big(\boldsymbol{H}(t), \boldsymbol{E}(t)\big) - \big(\boldsymbol{H}_h(t), \boldsymbol{E}_h(t)\big) \big\|_{L^2(Q)^6} \lesssim h^k,$$

with a constant independent of h. The key idea in the proof is to use the abstract extension $\mathcal{L}\boldsymbol{J}_\Sigma$ from the wellposedness result and to derive error bounds first for the shifted discrete field $\boldsymbol{H}_h - \pi_h \mathcal{L}\boldsymbol{J}_\Sigma$ with the L^2-projection π_h. We emphasize that this is only a theoretical tool, and $\mathcal{L}\boldsymbol{J}_\Sigma$ is not required for the implementation.

Since the discrete lift $\mathcal{L}_h \boldsymbol{J}_\Sigma$ appears as a volume current in the discrete system, we can in principle apply any time integration scheme to (2). For example, we can use the leapfrog method to obtain the fully discrete approximations

$$\begin{aligned}
\boldsymbol{H}_h^{n+1/2} &= \boldsymbol{H}_h^n - \frac{\tau}{2} \operatorname{curl}_{0,h} \boldsymbol{E}_h^n, \\
\boldsymbol{E}_h^{n+1} &= \boldsymbol{E}_h^n + \operatorname{curl}_h \boldsymbol{H}_h^n - \frac{\tau}{2} \mathcal{L}_h \big(\boldsymbol{J}_\Sigma^n + \boldsymbol{J}_\Sigma^{n+1}\big), \\
\boldsymbol{H}_h^{n+1} &= \boldsymbol{H}_h^{n+1/2} - \frac{\tau}{2} \boldsymbol{E}_h^{n+1},
\end{aligned}$$

for $n \geq 0$. Similarly, if the solution $\big(\boldsymbol{H}, \boldsymbol{E}\big)$ of (1) has piecewise Sobolev regularity $k+1$ in space and a bounded third time-derivative in $L^2(Q)^6$, we obtain under a CFL condition that for $n \in \mathbb{N}$ with $0 \leq t_n \leq T$ it holds

$$\big\| \big(\boldsymbol{H}(t_n), \boldsymbol{E}(t_n)\big) - \big(\boldsymbol{H}_h^n, \boldsymbol{E}_h^n\big) \big\|_{L^2(Q)^6} \lesssim h^k + \tau^2,$$

with a constant independent of h and τ.

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Exceptional points meet Nonlinear Dynamics

Alejandro Giacomotti

In this talk I've shown what exceptional points (EP) become in the nonlinear dynamical realm. For that I used a twofold approach: the realization of EPS in an experimental platform, and systematic comparison of the results with nonlinear dynamical models. The optical platform is nanophotonic cavities in semiconductor materials, which are coupled through evanescent waves

$$a_1 \longleftrightarrow a_2 \tag{1}$$

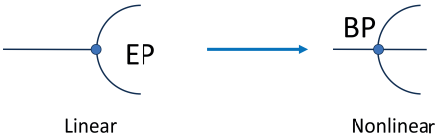
with κ the coupling. This system can be modeled with monlinear Hamiltonian equations

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = H \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \tag{2}$$

with

$$W = \begin{pmatrix} (w_1 + \kappa g_1) + i g_1 & \kappa \\ \kappa & (w_2 + \kappa g_2) + i g_2 \end{pmatrix}, \begin{cases} g_1 = g_1(a_1) \\ g_2 = g_2(a_2) \end{cases} \tag{3}$$

The EPS in the linear realm become bifurcation points of the NL dymamical system:



Proximity to NL EPs enables a wealth of NL dynamical Phenomena such as self-pulsin dynamics leading to frequency combs.

Local time-stepping methods for Friedrichs' systems

Marlis Hochbruck
(joint work with Constantin Carle, Malik Scheifinger)

Abstract

We consider local time-stepping methods for a general class of Friedrichs' systems employing a two-field structure, e.g., the linear Maxwell equations. For the space discretization we employ a discontinuous Galerkin method. We are interested in the particular situation that the spatial mesh has only a few fine elements since this leads to a strong CFL condition in explicit time integration schemes. Our main contribution is a new scheme which uses the leapfrog method on the coarse elements and the leapfrog-Chebyshev method on the fine elements.

1. Discontinuous Galerkin space discretization

Local time-stepping methods are very efficient in applications where the grid induced stiffness results from a few elements only. An extended overview on the literature can be found in [2] and [3]. For linear Maxwell equations such methods have been proposed in [5]. In our short presentation we consider local time-stepping methods for the more general class of two-field Friedrichs' systems. Special cases are linear Maxwell, acoustic wave or advection equations; see [4, Section 9.3] for details.

The discretization of a Friedrichs' system in space by a central fluxes discontinuous Galerkin (dG) approximation leads to

$$\begin{aligned} \partial_t u_h &= \mathcal{L}_{v,h} v_h + g_h, && \text{on } \mathbb{R}_+, \\ \partial_t v_h &= \mathcal{L}_{u,h} u_h, && \text{on } \mathbb{R}_+, \\ u_h(0) = \pi_h u^0, &\quad v_h(0) = \pi_h v^0, \quad g_h = \pi_h g \end{aligned} \tag{1}$$

where π_h denotes the L^2-orthorgonal projection onto the piecewise polynomial approximation space of the dG discretization and $\mathcal{L}_{u,h}$, $\mathcal{L}_{v,h}$ denote the discrete Friedrichs' operators. More details and properties can be found in [4, Chapter 10].

2. Local time integration

The leapfrog / Störmer–Verlet method is still the method of choice to integrate (1) in time numerically. Because we are interested in a mesh with a few fine elements, the leapfrog method suffers from a strict CFL condition. Here we follow [3] and propose to combine the leapfrog method with the leapfrog-Chebychev method [1].

For this we decompose the mesh $\mathcal{T} = \mathcal{T}_{h,\mathrm{lf}} \dot\cup \mathcal{T}_{h,m}$ into two submeshes, where $\mathcal{T}_{h,m}$ denotes the set of all elements $K \in \mathcal{T}$ which have a small diameter or which share a face with a small element, and $\mathcal{T}_{h,\mathrm{lf}} = \mathcal{T} \setminus \mathcal{T}_{h,m}$, see [4, Section 11.4] for details. Note that in [4], the notation $\mathcal{T}_{h,e}$ and $\mathcal{T}_{h,i}$ instead of $\mathcal{T}_{h,\mathrm{lf}}$ and $\mathcal{T}_{h,m}$, respectively, is used. With χ_m we denote the cutoff operator defined via

$$(\chi_m v)|_K = \begin{cases} v|_K, & K \in \mathcal{T}_{h,m}, \\ 0, & K \in \mathcal{T}_{h,\mathrm{lf}}. \end{cases}$$

A general class of local time-integration schemes can be constructed by means of a suitable filter function $\widehat{\Psi} : \mathbb{R}_0^+ \to \mathbb{R}$ which satisfies $\widehat{\Psi}(0) = 1$, see [2] for details. Given a timestep size $\tau > 0$ and approximations $u_h^n \approx u_h(t_n)$ and $v_h^n \approx v_h(t_n)$, the next timestep is given by

$$v_h^{n+1/2} - v_h^n = \frac{\tau}{2} \mathcal{L}_{u,h} u_h^n, \tag{2a}$$

$$u_h^{n+1} - u_h^n = \tau \widehat{\mathbf{\Psi}} \left(\mathcal{L}_{v,h} v_h^{n+1/2} + g_h^{n+1/2} \right), \tag{2b}$$

$$v_h^{n+1} - v_h^{n+1/2} = \frac{\tau}{2} \mathcal{L}_{u,h} u_h^{n+1}, \tag{2c}$$

with

$$\widehat{\mathbf{\Psi}} = \hat{\Psi}\left(-\tau^2 \mathcal{L}_{v,h} \chi_m \mathcal{L}_{u,h}\right). \tag{2d}$$

For $\widehat{\Psi} \equiv 1$, this is just the leapfrog scheme applied on all mesh elements. The choice of $\widehat{\Psi}(z) = (1 + z/4)^{-1}$ yields the locally implicit scheme considered and analyzed in [4, Sections 11.4 and 12.4]. A local time-stepping scheme is obtained by setting

$$\widehat{\Psi}(z) z = 2 - \frac{2}{T_p(\nu)} T_p\Big(\nu - \frac{z}{\alpha_p}\Big), \qquad \alpha_p = 2\frac{T_p'(\nu)}{T_p(\nu)}, \qquad \nu \geq 1. \tag{2e}$$

Here, T_p denotes the pth Chebyshev polynomial of first kind and $\nu \geq 1$ is a suitable chosen stabilization parameter, see [1, 2] for a discussion on the choice of ν.

3. Implementation

For an efficient implementation of the local time-stepping scheme (2) for $p \geq 2$, the essential step is the evaluation of $\widehat{\mathbf{\Psi}} c[test]_h$ with $\widehat{\mathbf{\Psi}}$ defined in (2d) and (2e). As in [1, Section 5.6], we define an auxiliary polynomial Υ of degree $p-2$ via

$$\widehat{\Psi}(z) = 1 + z\Upsilon(z).$$

By expanding the polynomial into the monomial basis and using $\chi_m^2 = \chi_m$, one observes

$$\begin{aligned}\widehat{\mathbf{\Psi}} w_h &= w_h - \tau^2 \mathcal{L}_{v,h}\chi_m \mathcal{L}_{u,h} \Upsilon\left(-\tau^2 \mathcal{L}_{v,h}\chi_m \mathcal{L}_{u,h}\right) w_h \\ &= w_h - \tau^2 \mathcal{L}_{v,h}\chi_m \Upsilon\left(-\tau^2 \chi_m \mathcal{L}_{u,h}\mathcal{L}_{v,h}\chi_m\right) \chi_m \mathcal{L}_{u,h} w_h\end{aligned}$$

Moreover, Υ satisfies a three-term recurrence relation obtained from that of Chebyshev polynomials, cf. [1, Lemma 5.30] and Algorithm 1.

Using the matrix representation of the discrete operators in the standard piecewise polynomial basis of discontinuous Galerkin methods, the cutoff operator is a diagonal matrix with only ones and zeros on the diagonal, referring to degrees of freedom (dofs) in mesh elements in $\mathcal{T}_{h,m}$ and $\mathcal{T}_{h,\mathrm{lf}}$, respectively. This shows that it is sufficient to compute only the few dofs of $\chi_m \mathcal{L}_{u,h} w_h$ corresponding to $\mathcal{T}_{h,m}$ (which means that only a few lines of the matrix representing $\mathcal{L}_{u,h}$ are required). Next, the matrix $\mathbf{A}_m$ representing $\chi_m \mathcal{L}_{u,h}\mathcal{L}_{v,h}\chi_m$ is of small size resulting in matrix-vector multiplications with short vectors only. A similar argument shows that $\mathcal{L}_{v,h}\chi_m$ can be computed efficiently.

The following algorithm to compute $\Upsilon(-\tau^2 \mathbf{A}_m)\mathbf{v}$ is taken from [1, Algorithm 5.2] (with a small typo corrected). Here, the coefficients $T_k(\nu)$ and α_k, $k = 1, \dots, p$, defined in (2e) can be precomputed by a three-term recurrence.

Algorithm 1 Computation of $\mathbf{w} = \Upsilon(-\tau^2 \mathbf{A}_m)\mathbf{v}$

$\mathbf{w}_0 = 0,\ \mathbf{w}_1 = -\frac{4}{\alpha_p^2 T_2(\nu)}\mathbf{v}$
for $k = 2, \dots, p-1$ **do**
  $\widetilde{\mathbf{w}}_{k-1} = -\tau^2 \mathbf{A}_m \mathbf{w}_{k-1}$
  $\mathbf{w}_k = 2\nu \frac{T_k(\nu)}{T_{k+1}(\nu)}\mathbf{w}_{k-1} - \frac{2}{\alpha_p}\frac{T_k(\nu)}{T_{k+1}(\nu)}\left(\frac{\alpha_k}{\alpha_p}\mathbf{v} - \widetilde{\mathbf{w}}_{k-1}\right) - \frac{T_{k-1}(\nu)}{T_{k+1}(\nu)}\mathbf{w}_{k-2}$
end for
$\mathbf{w} = \mathbf{w}_{p-1}$

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Response strength computation at higher-order exceptional points

Julius Kullig
(joint work with Jan Wiersig)

Non-Hermitian physics: Standard textbook quantum mechanic assumes the Hamiltonian of the system to be Hermitian such that real energy eigenvalues are ensured. That fundamental line of thought has been reconsidered by C. Bender and S. Boettcher [1] as they constructed a Hamiltonian $H = p^2 + V(q)$ that is non-Hermitian, possesses a parity($\mathcal{P}$)-time($\mathcal{T}$) symmetry, i.e. $[H, \mathcal{PT}] = 0$, and has a real spectrum. However, the considered potential $V(q) = iq^3$ is complex making it hard to implement as a traditional potential of a particle. Non-Hermitian photonics, however, gave an ideal platform for realization as the potential can be identified with the refractive index $n(\vec{q})$ where the imaginary part of $n(\vec{q})$ has a direct interpretation as gain/loss. Hence, a $\mathcal{PT}$-symmetric potential can be realized with coupled waveguides one with gain the other with loss [2]. Such a system is well described within coupled mode theory by a complex 2×2-matrix.

Exceptional points: In contrast to a system described by an Hermitian Hamiltonian the eigenvectors of a non-Hermitian Hamiltonian do not need to be orthogonal. In fact, changing the parameters of a non-Hermitian system can result in a defective Hamiltonian where not only the eigenvalues become degenerate but simultaneously also the corresponding eigenstates coalesce [3]. Typically this behavior relies on fine-tuning of system parameters which is why such non-Hermitian degeneracies are also called exceptional points (EPs). Around the EP the eigenvalues exhibit the characteristic topology of a complex root. Therefore small perturbations to the EP can result in a huge eigenvalue splitting which can be advantageous for sensors [4].

Waveguide-coupled microring cavities: Already passive optical systems are intrinsically non-Hermitian due to radiation. Therefore, the clockwise (CW) and counter-clockwise (CCW) propagating waves in a microring cavity have complex frequencies Ω with the imaginary apart of Ω describing the temporal decay. Zhong *et al.* [5] have shown that an attached waveguide with a mirror at one end results in asymmetric backscattering between CW and CCW waves of the microring. This immediately leads to an defective 2×2 Hamiltonian for the CW and CCW waves such that the system exhibits an EP of second order where two eigenstates coalesce. The order of the EP can be increased by adding more cavities to the waveguide such that each CW wave in one cavity only couples to the CW wave of the next cavity and vice versa for CCW waves [6]. In combination with the mirror at the waveguide's end this results in a EP of order $2N$ where N is the number

of cavities coupled via the waveguide. The intuitive approach via an effective $2N\times2N$ Hamiltonian is verified with full numerical COMSOL-simulations of the quasi-two-dimensional dielectric structure.

Response strength of exceptional points: Perturbing a system at an EP of order n with a generic perturbation ϵH_1 results in an eigenvalue splitting that scales with the nth root of ϵ. Beside this scaling it is possible to quantify the potential splitting near an EP by a response strength ξ that is independent of ϵ and H_1. This ξ defines an upper bound for the splitting via [7]

$$|\Omega_i - \Omega_{\mathrm{EP}}|^n \leq \epsilon \|H_1\|_2 \xi$$

where $\|\cdot\|_2$ denotes the spectral norm and Ω_i (Ω_{EP}) is the eigenfrequency of the perturbed (unperturbed) system. The computation of ξ, however, assumes that the Hamiltonian is given in matrix form. For a dielectric structure where the eigenstates (modes) are the time-harmonic solutions of Maxwell's equations the computation of ξ is not straightforward. However, we demonstrate a practical method of the numerical computation of ξ based on the Petermann factor which measures the overlap between left and right eigenstates of the system [8]]. This overlap can be calculated in COMSOL via numerical integration from the simulated electromagnetical fields. The approach is verified at waveguide-coupled mirroring cavities with mirror-induced asymmetric backscattering where the effective Hamiltonian is extracted from COMSOL simulations.

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Polarized high-frequency wave propagation beyond the nonlinear Schrödinger approximation

Christian Lubich

(joint work with Julian Baumstark, Tobias Jahnke)

The talk was about highly oscillatory solutions to a class of systems of semilinear hyperbolic equations with a small parameter $0 < \epsilon \ll 1$ for vector-valued solutions $u(t,x) \in \mathbf{R}^n$

$$\partial_t u + \sum_{\ell=1}^{d} A_\ell \partial_\ell u + \frac{1}{\varepsilon} E u = \varepsilon\, T(u,u,u), \qquad x \in \mathbf{R}^d,\ t \in [0, tend/\varepsilon] \tag{1}$$

$$u(0,x) = p(x) e^{i(\kappa\cdot x)/\varepsilon} + c.c. + O(\varepsilon) \tag{2}$$

with symmetric real $n \times n$ matrices $A_1, \dots, A_d$ and a skew-symmetric real $n \times n$ matrix E. On the right-hand side, $T : \mathbf{R}^n times \mathbf{R}^n times \mathbf{R}^n \to \mathbf{R}^n$ is a trilinear nonlinearity. This problem class includes, e.g., the Maxwell–Lorentz system and Klein–Gordon systems.

In the approximate initial condition, $\kappa \in \mathbf{R}^d \setminus \{0\}$ is a fixed wave vector and $p : \mathbf{R}^d \to \mathbf{R}^n$ is a smooth envelope function.

The interest here is in solutions that are polarized in the sense that up to a very small error, the oscillations in the solution depend on only one of the frequencies that satisfy the dispersion relation with the given wave vector $\kappa \in \mathbf{R}^n$ appearing in the initial wave packet. The construction and analysis of such polarized solutions is done using modulated Fourier expansions. This approach includes higher harmonics and yields approximations to polarized solutions that are of arbitrary order in the small parameter, going well beyond the known first-order approximation via a nonlinear Schrödinger equation. The given construction of polarized solutions is explicit and uses in addition a linear Schrödinger equation for each further order of approximation. Moreover, this construction is accessible to direct numerical approximation.

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Pseudospectra and non-normality in non-Hermitian Photonics

Kostas G. Makris

Abstract: One of the intriguing features of non-Hermitian photonics is the non-normal character of actual optical systems. We are going to present a unified framework for the systematic description of both extreme power dynamics and ultrasensitivity in terms of pseudospectra. The first part is devoted to recent results regarding a systematic way of characterizing the sensitivity around exceptional points in finite and infinite non-Hermitian topological lattices. In the second part

of the talk, we are going to examine the effect of transient power growth and amplification in dissipative optical waveguide lattices, again in terms of pseudospectra.

In the framework of non-Hermitian photonics [1], we present results [2-4] that are related to higher order exceptional points (HEP) in waveguide lattices. More specifically, in the first part of the talk, we propose a systematic methodology that allows us to characterize the extreme sensitivity of an optical system that operates around HEPs, based on pseudospectra theory, such as finite waveguide lattices and non-Hermitian Su-Schrieffer-Heeger (NHSSH) topological lattices [1]. The interplay between topological robustness, sensitivity and extreme amplification is also investigated by employing the pseudospectra theory [2]. Pseudospectra is a non-perturbative computational approach, that is widely used in fluid mechanics stability problems, and we introduced it in the context of optical physics and photonics. In the second part of this talk, we are going to examine the counter-intuitive phenomenon of transient growth despite the purely dissipative spectrum [5-7]. Pseudospectra can provide bounds based on Kreiss matrix theorem. Based on such a mathematical formalism, one can systematically investigate the extreme power dynamics and the determine the optimal geometric distribution of gain in an otherwise dissipative optical lattice [5-7]. We believe that our results may provide an important connection of exceptional points physics to non-Hermitian topological photonics [1,3,4].

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Stability and asymptotic properties of a linearized hydrodynamic medium model for dispersive media in nanophotonics

Serge Nicaise and Claire Scheid

Nanophotonics is the field that manages to exploit the interaction of light with nanometer scaled structures. With, nowadays, the ability of designing nanometer scaled devices, came the exponential growth of potential applications of nanophotonics. Subwavelength imaging is one of the famous example see *e.g.* [7, 2] and references therein. Most of very interesting features in nanophotonics come from

the possibility to enhance fields leading to the creation of very good absorbers or emitters (see one example in *e.g.* [2, 11, 6]). All these reasons make nanophotonics a very active field of research. Nanoplasmonics, one of the major subfield of Nanophotonics is of particular interest. It is based on the exploitation of plasmons (see [5] for a physical insight). These occur when the light interact with nanoscaled *metals*. Modelling is at the heart of the understanding of nanoplasmonics. It relies on the description of the reaction of the electrons of the metal to an applied external electric field. Popular classical models rely on a mechanical description of the movement of the electrons. These descriptions lead to the famous Drude and Drude-Lorentz models that are describing the electric dispersive nature of metals at optical frequencies. Indeed, electrons exhibit a delay in response to the applied electric field and a polarization that characterizes a dispersive media. These models give very good results when the size of the device is not smaller than $\simeq 15nm$. Below this threshold, the repulsive interaction between electrons in the metal do play an important role. Models that take into account of these effects are called "non-local" in the sense that the reaction of the electron not only depends on the applied electric field at its precise position but also on the field around it. To model these effects, one can describe the metal as a fluid of electron and makes use of a hydrodynamical description (see [1]). This is the point of view that we have adopted, focusing on the linear response of such systems. The equations that we consider come from a linearization of the non linear hydrodynamical model around a static equilibrium. The resulting system write formally as:

$$\left\{\begin{array}{l} \varepsilon_0\varepsilon_L\partial_t E - \mathrm{rot}H = -J, \\ \mu\partial_t H + \mathrm{rot}E = 0, \\ J_{tt} + \gamma\partial_t J - \beta^2\nabla(\mathrm{div}J) = \varepsilon_0\omega_p^2\partial_t E, \end{array}\right. \tag{1}$$

This system is a linear hyperbolic system of PDE's that encompass the "non-local" character of the response through a linearized quantum pressure term and consists in a linear coupling between Maxwell's equations (with (E, H) the electromagnetic field) with a PDE that describes the evolution of the polarization current J. Classically, ε_0, the vacuum permeability, ε_L, the relative permeability of the media and μ, its permittivity, are physical constants. Furthermore, ω_p^2 is the plasma frequency and β is the so-called "nonlocal" parameter. One should notice that if $\beta = 0$, the system (1) reduces to Drude dispersive model that has been investigated numerically in [3] (with Nédélec elements), [9, 10] (with a Discontinuous Galerkin framework) with an emphasis on computational aspects; the benefit for nanoplasmonics has been shown. However, no theoretical study of the continuous model has been provided. Physicists are still debating on the right boundary condition to impose to the system, basing their arguments on natural physical considerations. In [4], well posedness has been investigated for (1), with zero normal trace for J current, using variational techniques and without considering charge conservation that is inherent to this system. In this work, we first investigate the question of well posedness for several types of boundary conditions with the point of view of semigroup theory and including charge conservation. Stability is an important

feature with regards to the complete understanding of the phenomenon and has also an impact on the development of adapted numerical frameworks. We thus also propose to investigate polynomial stability and optimal polynomial decay. This has been studied in details for all classical dispersive media in [8] but not for the more involved system (1) for which we have extended the latter results. We are also concerned with the behavior of numerical schemes with respect to (polynomial) stability using the Discontinuous Galerkin discretization framework of [9] combined with several explicit time integration schemes in 2D (from Leap-frog to explicit Runge-Kutta schemes). Furthermore, we prove that the charge constraint inherent to (1), is weakly preserve at the discrete level.

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Non-Hermitian Optics and Photonics

Ramy El-Ganainy

In this talk, I will give a survey over the field of non-Hermitian optics and photonics. I will start by first explaining the notions of parity and time reversal symmetries followed by a brief introduction to the seminal work of Bender. et.al. that showed that PT symmetric Hamiltonians can have real spectra. The formal analogy between the single particle Schrodinger equation and the paraxial equation of diffraction will be then used to introduce the concept of PT symmetry in optics. Implementations of PT symmetry using coupled waveguides and cavities

will be then discussed. An important concept related to non-Hermitian physics is that of exceptional points (EPs). In this talk, I will introduce the notion of EPs together with their implementations using PT symmetry and unidirectional coupling between degenerate optical modes in microring resonators. Finally, I will discuss briefly some applications of non-Hermitian optics and laser engineering and sensing.

The effect of bound states of nearly free electrons on the propagation of intense ultrashort light pulses in gases

Maria Richter

(joint work with Felipe Morales, Serguei Patchkovskii, Mary Matthews, Alexander Patas, Albrecht Lindinger, Julien Gateau, Nicolas Berti, Sylvain Hermelin, Jérome Kasparian, Timm Bredtmann, Olga Smirnova, Jean-Pierre Wolf, Anton Husakou, and Misha Ivanov)

Since the late 1980s, it has been speculated that when an atom or molecule interacts with an intense light field, whose strength substantially exceeds the ionic Coulomb attraction, new and surprisingly stable states of a hybrid quantum system, "atom + intense light field", can be formed [1]. The electron becomes nearly but not completely free: rapidly oscillating in the laser field, it still feels residual attraction to the core, which keeps it bound [1,2]. These exotic states are known as the Kramers-Henneberger (KH) states [3], a specific example of laser-dressed states [2]. It took three decades before the existence of such states was indirectly inferred from experiments [2], showing the ability of isolated neutral atoms to survive laser intensities as high as $I \sim 10^{15} - 10^{16}$ W/cm^2.

But are such unusual stable states really exotic? Can they also form in gases at ambient conditions, at intensities well below 10^{15-16} W/cm^2? After all, for excited electronic states bound by a few eV, the laser field overpowers the Coulomb attraction to the core already at $I \sim 10^{13-14}$ W/cm^2. If this is the case, would these exotic stable states manifest inside laser filaments [4]?

The formation of the KH states should modify both real [5] and imaginary parts [6] of the refractive index of a laser-driven system. While their response is almost free-electron-like, they do form discrete states and lead to new resonances. Qualitatively, these resonances can be understood as Stark-shifted field-free states, with stability against ionization being their key distinguishing feature. Crucially, at sufficiently high intensities theory predicts the emergence of population inversion in the higher Rydberg states relative to the lowest excited states [7]. This inversion reflects the increased stability of the KH states and is the signature of the transition into the stabilization regime. If the inversion were created inside a laser filament, it would lead to amplification of the filament spectrum at the transition frequencies between the stabilized states.

We describe a combination of experimental and theoretical results [8], which show that the KH states arise not only in isolated atoms, but also in rare gases at and above atmospheric pressure, where they can act as a gain medium during

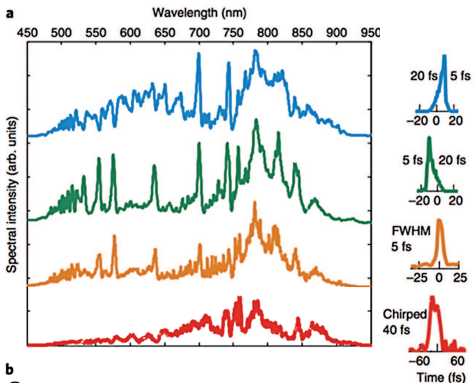

FIGURE 1. Forward emission spectra from different pulse shapes filamenting in argon at 9 bar. Gaussian pulse shape with 40 fs duration, a 7 fs Fourier-limited pulse, a sawtooth shaped pulse, where the sharp front (5 fs) arrives first, afollowed by a trailing 20 fs decay, and the reversed sawtooth with 20 fs rise and 5 fs decay time. Spectra of pulses with sharp fronts (yellow and green) exhibit emission lines (see spectrum around 500-600 nm) characteristic of the laser-dressed atom.

laser filamentation. Using shaped laser pulses with sharp rise times, gain in these states can be achieved within just a few cycles of the guided field, leading to amplified emission in the visible, at lines peculiar to the laser-dressed atom. Fig. 1 shows the experimentally measured forward emission from different pulse shapes filamenting in argon at 9 bar with the same spectra, but different temporal shapes. The smooth Gaussian pulse (red line) yields a typical supercontinuum spectrum, with no resonant lines attributable to atoms or ions. When the pulse rise is fast (orange and green lines), we observe dramatically different spectra with distinct asymmetric, Fano-like amplification lines between 530 and 625 nm, as predicted by the theory.

To further elucidate the effect of population inversion dynamics during fs laser filamentation, we have developed a first-principle model [9,10] for the accurate simulation of spatio-temporal light pulse dynamics based on the solution of a (2+1)D unidirectional pulse propagation equation (UPPE). At each propagation step, the system's (highly nonlinear) response is provided by the solution of the 3D time-dependent Schrödinger equation (TDSE). The model goes beyond the standard SFA-like approximation of the system's response and accounts for the laser-dressed multilevel structure of the system, including the bound and the free states, the system's subcycle response, and the feedback of the generated light to the IR driver. Femtosecond laser filamentation simulations for atomic hydrogen indeed reveal the generation of population inversion that persists throughout the pulse propagation distance and that leads to a new emission peak in the spectrum.

Our work suggests that the unusual, laser-dressed, stable states of neutral atoms can be exploited to create a general, new, ultrafast gain mechanism during laser filamentation.

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Nonlinear optical response of crystalline metal films

Álvaro Rodríguez Echarri, Kurt Busch
(joint work with Javier García de Abajo, Joel D. Cox)

Nanoscale nonlinear optics is limited by the inherently weak nonlinear response of conventional materials and the small light-matter interaction volumes available in nanostructures. Plasmonic excitations can alleviate these limitations through subwavelength light focusing, boosting optical near fields that drive the nonlinear response, but also suffering from large inelastic losses that are further aggravated by fabrication imperfections. Here, we theoretically explore the enhanced nonlinear response arising from extremely confined plasmon polaritons in few-atom-thick crystalline noble metal films. Our results are based on quantum-mechanical simulations of the nonlinear optical response in atomically thin metal films that incorporate crucial electronic band structure features associated with vertical quantum confinement, electron spill-out, and surface states. We predict an overall enhancement in plasmon-mediated nonlinear optical phenomena with decreasing film thickness, underscoring the importance of surface and electronic structure in the response of ultrathin metal films.

Numerical modelling of dispersive media

Claire Scheid

(joint work with A. Gobé, S. Lanteri, A. Moreau, S. Nicaise, N. Schmitt and J. Viquerat)

Exploiting the optical response of metallic nanostructures illuminated by light allows to overcome the diffraction limit of classical optics. Efficient and extreme confinment of light can be achieved, thanks to the existence of plasmonic waves (especially at metallo-dielectric interfaces)[1]. One thrilling consequence is that the design of very good light emitters or absorbers is then at reach. In order to assess or infer the performance of possible structures, an accurate numerical modelling of the optical response of metallic nanostructures is crucial. In this talk, we focus on the linear optical response in nanoplasmonics. We propose to review the classical models used and describe a complete numerical framework in this context.

The propagation of light in a given medium is modelled with the set of Maxwell's equations as folllows

$$\frac{\partial D}{\partial t} = \mathrm{curl} H,\ \frac{\partial B}{\partial t} = -\mathrm{curl} E. \tag{1}$$

Here E and H are resp. the electric and magnetic fields, D and B are resp. the electric displacement and magnetic induction. The characteristics of the media in which the light propagates is encoded in the constitutive relations. In usual linear dielectric media, $D = \varepsilon_0 \varepsilon_r E$, $B = \mu_0 \mu_r H$. Here ε_0 (ε_r) is the vacuum (relative) permittivity, and μ_0 (μ_r) the vacuum (relative) permability. We consider non magnetic media so that $\mu_r = 1$. In metallic media, the oscillations of the electron cloud of the metal create the so-called plasmonic waves. This optical response is in all generality nonlocally electrically dispersive. Whereas it can be neglected in many dielectric devices, the linear optical response of a lot of structures encountered in nanoplasmonics can be impacted by this nonlocality. This might occur in several ways: time nonlocality (the electrons of the metal react with a time delay to the electric excitation), space nonlocality (the reaction of the electron depends on the electric field in a vicinity of its position), a combination of the two above-mentioned phenomena. This electric dispersive character is then encoded in the electrical constitutive relation via a causal convolution in time and/or space ($\star_{t,x}$). Properties of the permittivity allows to decouple the local ($\varepsilon_0 \varepsilon_r E$) and the nonlocal ($P$, called a polarization vector) contributions in the consititutive relation $D = \varepsilon \star_{t,x} E = \varepsilon_0 \varepsilon_r E + P$. Inserting these relations into Maxwell's equations provides a new set of equations driving the evolution of the electric and magnetic field E and H, where the dispersive part is expressed through a so-called polarization current ($J = \dfrac{\partial P}{\partial t}$). This reads

$$\varepsilon_0 \varepsilon_r \frac{\partial E}{\partial t} = \mathrm{curl} H - J,\ \mu_0 \frac{\partial H}{\partial t} = -\mathrm{curl} E.$$

[1] oscillation of the electron cloud of the metal

Closing the model amounts to determining a model to describe the space-time evolution of this current J. Classical approaches to model nonlocality in time are based on oscillator type models (*e.g* Drude or Lorentz oscillators), and their combinations; the evolution of J (or P) is driven by a set of ODEs coupled to Maxwell's equation through the driving force $\omega_p^2 E$, where ω_p is the plasma frequency. On the other hand, spatial nonlocal effects, due to inter-electron pressure, can be extracted from the linearization of a hydrodynamic description of the electron cloud; an extension of the Drude model is obtained (the so-called linearized hydrodynamical Drude model). The latter is a linear hyperbolic PDE (hiding bulk plamonic waves) coupled to Maxwell's equations through a linearized Lorentz force (same driving force as in the Drude model).

The inherent structure of these various couplings[2] gives to the problem a natural decreasing physical energy. This quantity serves as a guideline for our works. First, in the theoretical analysis of the various models: well-posedness is at reach using classical linear semi-group theory. Moreover, precise stability estimates quantifying decay rates are achievable ([10, 7, 8]). Second, keeping track of the energy at the discrete level is crucial to characterize important properties of the numerical schemes (in particular stability). Desirable schemes would strive not to destroy the continuous energy principle or at least not to destroy it at convergence.

The challenges raised in nanoplasmonics, in particular by the characteristics of the media, and the various scales involved, require a suitable framework capable of dealing with them effectively. We propose to use non conforming finite elements for the approximation in space, namely discontinuous Galerkin Finite elements. Time integration is obtained using explicit schemes (such as Leap-frog or explicit Runge Kutta schemes). From the design of the schemes up to numerical academic simulation, we provide a quite complete study of this approach. These studies include in particular the stability and/or convergence (see *e.g.* [2, 1, 7]). As a result, we obtain a promising robust environment, assessed on academical contexts.

To tackle real problems, a sole academic study (even if necessary) is not sufficient. Indeed, concrete scenari involve several media and possibly complicated structures. As a simple example, in a typical setting, one or several metallic nanostructures are embedded in a dielectric environment and the structure is excited by a light source. The possible complexity of the setting calls for several enhancements ranging from improving the initial methodology (*e.g.* special type of sources, multi-scale/-element or curvilinear strategies, see *e.g.* [3, 4, 5]...) to specific post-treatment (*e.g.* quantities of interest, frequency spectrum...). Besides, a crucial question, that we address in this talk, is also whether these dispersive models are relevant, since it can be viewed as (possible unnecessary) refinements of dielectric models. The accuracy of time dispersive models in a wide range of nanoplasmonics structures is known for years. However, space-time dispersive (nonlocal) models are still questioned. Hence, being able to find a reasonnable (not so small) structure, for which space-time nonlocal effects are significantly impacting plasmonic resonances, is determinant. One especially expects that plasmons existing at a

[2]Maxwell's equations with either linear ODE's or PDE's.

metallo-dielectric interface (surface plasmons) are good candidates to be sensitive to space-time nonlocality. Indeed, one decisive observation is that if the permittivity of the dielectric at the interface increases, so does the sensitivity of surface plasmons to non-locality. As a consequence, even "large" nanoparticles (> 20 nm) are expected to be sensitive to spatial nonlocality [9], so that for any plasmonic structure in a high permittivity dielectric, spatial nonlocality should be taken into account. With this in mind, in [6] (collaboration with Institut Pascal, Clermont-Ferrand, France and TU Darmstadt, Germany), we studied the impact of spatial nonlocality on surface plasmons propagating at a metallo-dielectric interface, with a dielectric of high permittivity (TiO_2, Titanium dioxide), for a simple metallic grating allowing the excitation of surface plasmons. We set up a procedure to measure the signature of spatial dispersion precisely by tracking the surface plasmons resonances in the reflection spectrum of the structure. In particular, we have illustrated the influence of a variation of geometrical parameters of the grating structure for a given surface plasmon resonance mode. Our numerical results confirm that the resonance shift can be clearly attributed to spatial nonlocal effects.

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The NLS equation and modulating pulses in Nonlinear Optics

Guido Schneider

We consider dispersive nonlinear models of Nonlinear optics. The simplest such model is the cubic Klein-Gordon (cKG) equation

$$\partial_t^2 u = \partial_x^2 u - u + u^3,$$

with $x, t, u(x,t) \in \mathbb{R}$. Making the ansatz

$$u(x,t) = \varepsilon A(\varepsilon(x - c_g t, \varepsilon^2 t) e^{i(k_0 x - \omega_0 t)} + c.c. + \mathcal{O}(\varepsilon^3),$$

with $0 < \varepsilon^2 \ll 1$ a small perturbation parameter, and equating the coefficient in front of $\varepsilon^3 e^{i(k_0 x - \omega_0 t)}$ to zero gives an NLS equation

$$-2i\omega_0 \partial_T A = (1 - c_g^2)\partial_X^2 A + 3A|A|^2,$$

describing slow modulations in time and space by the envelope A, moving in the laboratory frame with group velocity c_g, of the underlying carrier wave $e^{i(k_0 x - \omega_0 t)}$. For in introduction in geometric or nonlinear optics see [1].

Approximation results guarantee that the NLS equation makes correct predictions about the dynamics of the original system on the natural NLS time scale. Such results are easily established in case that the original system has no quadratic terms. If quadratic terms are present these have to be eliminated with normal form transformations or averageing. In order to do so, non-resonance conditions have to be satisfied. By perturbation theory the interaction dynamics can be separated from the internal dynamics of two NLS scaled wave packets up to high order. For an overview see [2, 3].

In spatially periodic media the carrier waves are time-harmonic Bloch modes instead of time-harmonic Fourier modes. The approximation theory for the spatially homogeneous case can be transferred to the spatially periodic case, cf. [4].

In nonlinear optics the role of time and space very often is interchanged. A spatially periodic medium transfers into a time-periodic medium. For time-periodic systems like Hill's equation or Mathieu's equation it is well known that large instability regions occur. The validity and in particular the non-validity of the NLS approximation in time-periodic media is discussed in [5]. Moreover, the non-validity of the dispersion management equation is discussed in [5], too.

If 1-solitons instead of arbitrary solutions of the NLS equation are considered the approximation-time can be extended from an $\mathcal{O}(1/\varepsilon^2)$-time scale to an $\mathcal{O}(1/\varepsilon^N)$-time scale with N arbitrary large but fixed. The proof is based on spatial dynamics, invariant manifold theory and a finite speed of propagation. See [6] and for a recent result [7].

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Extremely Narrow, Sharp-Peaked Resonances at the Edge of the Continuum

Kestutis Staliunas

(joint work with I. Lukosiunas, L. Grineviciute, J. Nikitina, D. Gailevicius)

It is well known that the wavefunctions in a potential well can form bound states for their energies below the background of the potential well, and the continuum states for their energies above the background. Although the basic wave behavior in the potential wells has been established since the beginning of quantum mechanics, new findings are constantly being reported. One such example is the phenomenon of Bound States in the Continuum,. Here we report another effect never considered before – extreme sharpening of the peaks of the resonances when their energies approach the background energy of the potential well, just before crossing the boundary of the continuum.

The physical situation is depicted in Fig.1. The situation can be realized in thin, nano-modulated dielectric films, where the periodic modulation of the interface serves as a drive of the potential well. The situation mathematically can be described by an externally driven Schrödinger equation:

$$\frac{\partial^2 A_1(z)}{\partial z^2} + (E - V(z))\, A_1(z) - i\gamma(z) e^{ik_{0,z} z} A_0(z) = 0$$

The $\gamma(z)$ is the normalized coupling profile, see Fig. 1, $V(z)$ is the profile of the potential (corresponding to the refraction index profile in optics), and E is the position of the driving ion the energy (frequency) domain (corresponds to frequency of excitation in optics). When the energy of the driving force is below the edge of the continuum, the usual discrete resonances are excited. These are Fano resonances with their typical (asymptotically Lorenz-like) form [2]. However when the potential is deformed so, that one of the resonances approaches the edge of a continuum, a critical sharpening of the resonance is observed. The usual Lorentzian-like shapes, which asymptotically at around their peaks follow

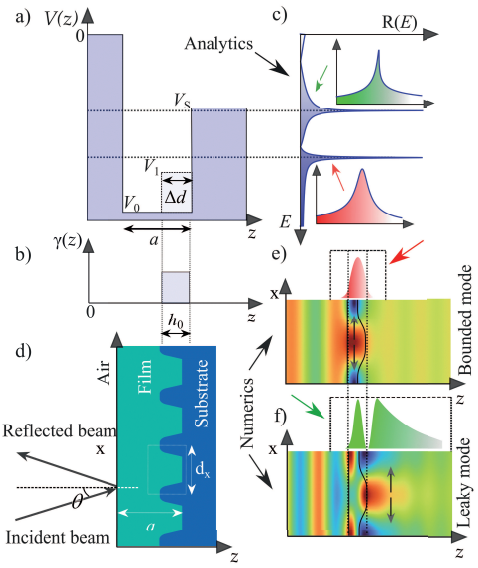

FIGURE 1. (a) A driven potential well (a,b) is equivalent to the thin film of high refraction index with periodically modulated interface (d). Mathematically driving is equivalent to imaginary part of the potential (b). The interface modulation couples the nearly-normal FP mode into the bounded waveguided modes (e) or leaky surface modes (f), resulting in the usual Lorenz-shaped resonance, or sharp-peaked resonances, respectively (c).

the parabolic law $1 - d\omega^2$, deforms into sharp-peaked ones with the asymptotical shapes of $1 - |d\omega|$. Also the scalings of the width of the resonance with the coupling parameter at the continuum boundary is different from the usual scalings of Fano resonances. We demonstrated such sharpening of the resonances also experimentally, in thin, nano-modulated dielectric films, We have discussed the possible realization of the effect in passive systems (the thin film on the dielectric substrate) as well as in active (the film on amplifying material).

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Introduction to numerical homogenization and application in nonlinear optics

Barbara Verfürth

Many applications include processes on different length scales. Mathematically, this leads to so-called multiscale problems where the coefficients in the PDE vary strongly on small spatial scales. Direct numerical simulations with, e.g., the finite element method require to resolve all involved scales, which is often computationally too demanding. In this contribution, we give a brief introduction to two different computational multiscale methods, which aim at the approximation of the macroscopic solution behavior. As an example, we consider the following elliptic multiscale problem written in weak form: Find $u \in H^1_0(\Omega)$ such that

$$b(u,v) := (a\nabla u, \nabla v) = (f,v),$$

where Ω is a bounded Lipschitz domain, $f \in L^2(\Omega)$, $a \in L^\infty(\Omega)$ bounded from above and below and entailing multiscale features as described above, and $(\cdot,\cdot)$ denotes the $L^2(\Omega)$-scalar product. Finally, we outline the application to a Helmholtz equation with Kerr nonlinearity.

1. The Heterogeneous Multiscale Method (HMM)

One prototypical example of a multiscale coefficient is the case where a is locally ε-periodic, i.e., it is of the form $a(x, \frac{x}{\varepsilon})$, where a is 1-periodic in the second argument. Such a coefficient varies on the scale $\varepsilon \ll 1$ and the finite element method would require a mesh size $H < \varepsilon$. Instead of directly approximating u, one considers the limit $\varepsilon \to 0$ using homogenization theory. In fact, u converges towards a unique $u_0 \in H^1_0(\Omega)$ in a suitable sense, where u_0 is again the solution to an elliptic problem, but with a homogenized, slowly varying coefficient a_0. Therefore, u_0 can be approximated by a finite element method on a coarse mesh with mesh size $H \gg \varepsilon$. However, the values of the homogenized coefficient a_0 still need to be computed, at least at the quadrature points. Since homogenization theory gives a_0 via the solution of additional PDEs (so-called cell problems) on the unit cell, one of the central ideas in the HMM is to approximate a_0 via the solutions of discretized cell problems. This is done on small ε-cells around the quadrature points. Further details on the HMM, in particular estimates of the discretization error, are found, e.g., in [1].

2. The Localized Orthogonal Decomposition (LOD)

While the HMM modifies the bilinear form b (via the use of the approximated homogenized coefficient), the LOD modifies the test and ansatz spaces to use problem-adapted multiscale basis functions instead of piecewise polynomials. Further, one directly aims to approximate the solution u of the multiscale problem instead of the homogenized solution u_0. Thereby, the LOD does not require the assumptions of local periodicity nor scale separation.

Let $\mathcal{T}_H$ denote a shape regular, quasi uniform triangulation of Ω which is coarse in the sense that it does not resolve the variations of a. The basis functions of the associated lowest-order Lagrange finite element space are denoted by λ_z, which are piecewise affine functions evaluating to 1 at vertex z of $\mathcal{T}_H$ and zero at all other vertices. The LOD is a Galerkin method based on the multiscale space

$$V_H^\ell := \operatorname{span}\{\Lambda_z^\ell : z \text{ vertex of } \mathcal{T}_H\} \quad \text{with} \quad \Lambda_z^\ell = \lambda_z - \sum_{T\in\mathcal{T}_H, z\in T} \mathcal{C}_{\ell,T}\lambda_z.$$

The multiscale basis functions Λ_z^ℓ are, hence, constructed as corrections to the finite element basis functions. Here, $C_{\ell,T}\lambda_z \in W(U_\ell(T))$ is the unique solution to

$$b(C_{\ell,T}\lambda_z, w) = b(\lambda_z|_T, w) \quad \forall w \in W(U_\ell(T)).$$

The underlying local finescale space $W(U_\ell(T))$ consists of all functions which (a) vanish outside the so-called ℓ-layer patch $U_\ell(T)$ and (b) are finescale in the sense that they lie in the kernel of a suitable, stable interpolation operator I_H, which is a projection onto the finite element space spanned by λ_z. The ℓ-layer patch $U_\ell(T)$ is defined inductively as the union of all elements T' that touch $U_{\ell-1}(T)$, where $U_0(T) = T$. Details on the construction of the LOD and estimates for the discretization error are found, e.g., in [2]. Importantly, the constants in the error bounds are independent of the variations of a and not more that H^1-regularity of the solution u is required to nevertheless obtain a convergence rate $O(H)$.

3. Application of the LOD in nonlinear optics

In [3], we designed and analyzed an LOD-inspired numerical multiscale method for the nonlinear Helmholtz equation: Seek $u \in H^1(\Omega)$ such that

$$b(u, v) := (a\nabla u, \nabla v) - k^2((n_0 + \chi_D n_2|u|^2)u, v) - ik(u, v)_{\partial\Omega} = (f, v),$$

where k is the wave number, a, n_0 and n_2 are multiscale coefficients and D is a compactly embedded subdomain on which the nonlinearity acts. Our adaptive iterative multiscale approximation combines three main ingredients:

(1) a fixed point iteration, where in each step a linear Helmholtz equation is solved with the nonlinearity $|u|^2$ evaluated based on the previous iteration;
(2) an LOD-type multiscale method in each iteration (cf. Section 2) applied to the linearized Helmholtz equation from the first point;
(3) an adaptive computation of the multiscale basis functions, so that $\mathcal{C}_{\ell,T}$ is newly calculated only if the nonlinearity changed significantly around T, based on a local error indicator.

We refer to [3] for further details on the construction and error estimates as well as for numerical experiments.

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Reporter: Álvaro Rodríguez Echarri

Participants

Dr. Heiko Appel
Max-Planck-Institut für Struktur und Dynamik der Materie
und Center for Free-Electron Laser Science (CFEL)
Luruper Chaussee 149
22761 Hamburg
GERMANY

Priv.-Doz. Dr. Uwe Bandelow
Weierstraß-Institut für Angewandte Analysis und Stochastik
Mohrenstr. 39
10117 Berlin
GERMANY

Prof. Dr. Weizhu Bao
Department of Mathematics
National University of Singapore
Lower Kent Ridge Road
Singapore 119 076
SINGAPORE

Prof. Dr. Kurt Busch
Theoretical Optics & Photonics
Institut für Physik
Humboldt-Universität Berlin
Lise-Meitner Haus
Newtonstr. 15
12489 Berlin
GERMANY

Dr. Christian Döding
Institut für Numerische Simulation
Universität Bonn
Friedrich-Hirzebruch-Allee 7
53115 Bonn
GERMANY

Dr. Benjamin Dörich
Institut für Angewandte und Numerische Mathematik
Karlsruher Institut für Technologie (KIT)
Englerstraße 2
76131 Karlsruhe
GERMANY

Julian Dörner
Institut für Angewandte und Numerische Mathematik
Karlsruher Institut für Technologie (KIT)
Englerstraße 2
76131 Karlsruhe
GERMANY

Prof. Dr. Ramy El-Ganainy
Dept. of Physics
Michigan Technological University
1400 Townsend Drive
Houghton, MI 49931
UNITED STATES

Dr. Alejandro Giacomotti
LP2N, Institut d'Optique Graduate School
CNRS, Université de Bordeaux
Rue François Mitterrand
33400 Talence
FRANCE

Prof. Dr. Marlis Hochbruck
Institut für Angewandte und Numerische Mathematik
Karlsruher Institut für Technologie (KIT)
Englerstraße 2
76131 Karlsruhe
GERMANY

Dr. Julius Kullig
Abteilung Theorie der kondensierten Materie
Institut für Physik (IfP)
Otto-von-Guericke-Universität Magdeburg
Universitätsplatz 2
39106 Magdeburg
GERMANY

Prof. Dr. Christian Lubich
Mathematisches Institut
Universität Tübingen
Auf der Morgenstelle 10
72076 Tübingen
GERMANY

Prof. Dr. Konstantinos Makris
University of Crete
Department of Physics
Voutes University Campus
70013 Heraklion
GREECE

Prof. Dr. Serge Nicaise
DMATHS, CERAMATHS
Université Polytechnique Hauts-de-France
Le Mont Houy
59313 Valenciennes Cedex 9
FRANCE

Dr. Maria Richter
Max-Born-Institut (MBI)
im Forschungsverbund Berlin e.V.
Max-Born-Straße 2A
12489 Berlin
GERMANY

Dr. Álvaro Rodríguez Echarri
Theoretical Optics & Photonics
Institut für Physik
Humboldt-Universität Berlin
Lise-Meitner Haus
Newtonstr. 15
and
Max-Born-Institut
12489 Berlin
GERMANY

Maximilian Ruff
Fakultät für Mathematik
Karlsruher Institut für Technologie (KIT)
Englerstraße 2
76131 Karlsruhe
GERMANY

Prof. Dr. Claire Scheid
Laboratoire J.-A. Dieudonné
Université Côte d'Azur
Parc Valrose
06108 Nice Cedex 02
FRANCE

Prof. Dr. Guido Schneider
Institut für Analysis, Dynamik und Modellierung
Fakultät für Mathematik und Physik
Universität Stuttgart
Pfaffenwaldring 57
70569 Stuttgart
GERMANY

Prof. Dr. Kestutis Staliunas
ICREA
Passeig Lluís Companys 23
08010 Barcelona
SPAIN

Prof. Dr. Barbara Verfürth
Institut für Numerische Simulation
Universität Bonn
Friedrich-Hirzebruch-Allee 7
53115 Bonn
GERMANY