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Efficient resonance computations for Helmholtz problems based on a Dirichlet-to-Neumann map

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ABSTRACT

We present an efficient procedure for computing resonances and resonant modes of Helmholtz problems posed in exterior domains. The problem is formulated as a nonlinear eigenvalue problem (NEP), where the nonlinearity arises from the use of a Dirichlet-to-Neumann map, which accounts for modeling unbounded domains. We consider a variational formulation and show that the spectrum consists of isolated eigenvalues of finite multiplicity that only can accumulate at infinity. The proposed method is based on a high order finite element discretization combined with a specialization of the Tensor Infinite Arnoldi method (TIAR). Using Toeplitz matrices, we show how to specialize this method to our specific structure. In particular we introduce a pole cancellation technique in order to increase the radius of convergence for computation of eigenvalues that lie close to the poles of the matrix-valued function. The solution scheme can be applied to multiple resonators with a varying refractive index that is not necessarily piecewise constant. We present two test cases to show stability, performance and numerical accuracy of the method. In particular the use of a high order finite element discretization together with TIAR results in an efficient and reliable method to compute resonances.

1. Introduction

In this paper we consider the numerical approximation of resonances in an open system, where the solutions satisfy the Helmholtz equation for a given refractive index $\eta(x)$. In general, resonances of an operator are defined as poles of the resolvent operator taken in a particular generalized sense [1,2]. For Helmholtz equation Lenoir et al. [3] have shown that resonances are solutions to a nonlinear eigenvalue problem (NEP) with a Dirichlet-to-Neumann (DtN) map $\mathcal{G}(\lambda)$ on an artificial boundary Γ. The pair (u, λ) is a scattering resonance pair if

$$\begin{aligned} \Delta u + \lambda^2 \eta^2 u &= 0 \qquad \text{in } \Omega, \\ \frac{\partial u}{\partial n} &= \mathcal{G}(\lambda) u \ \text{ on } \Gamma, \end{aligned} \tag{1}$$

where $\partial u/\partial n$ is the normal derivative and the non-negative function $\eta^2 - 1$ has compact support contained in the open domain Ω. Hence, although our differential operator (1) is linear in λ^2 the DtN operator $\mathcal{G}(\lambda)$ (which we formalize in Section 2) depends in a nonlinear way on the eigenvalue λ.

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The considered NEP is of the type: find $\lambda \in \mathbb{C}$ in an open subset of the complex plane and a non-zero $x \in \mathbb{C}^n$ such that

$$T(\lambda)x = 0. \tag{2}$$

In our case T is meromorphic in $\mathbb{C}$, with poles in the region of interest defined as scaled roots of Hankel functions. Many numerical methods for the NEP (2) have been developed in the numerical linear algebra community, in particular when T is holomorphic in a large domain. Since the NEP with an arbitrary normalization is a system of nonlinear equations, Newton's method can be applied and considerably improved, e.g., by using block variations that can compute several eigenpairs simultaneously [4]. However, Newton-type methods bear the danger that some eigenvalues close to a given target could be missed. There are also generalizations of successful methods for linear eigenvalue problems, e.g., the nonlinear Arnoldi method [5], the Jacobi–Davidson method [6] and LOBPCG [7]. Numerical methods for NEP can be based on contour integrals of the generalized resolvent $T^{-1}(\lambda)$ [8–12]. The DtN-map is the source of the complicated nonlinearity in the eigenvalue parameter λ. Several other problems have been approached with artificial boundary conditions and NEPs; see, e.g., the NEP arising in the modeling of an electromagnetic cavity [13], the model of an optical fiber in [14] and bi-periodic slabs [15]. There are also several approaches leading to NEPs developed in the context of photonic crystals [16–19]. To our knowledge, none of the methods developed in those papers have been adapted to resonance problems of our type.

Infinite Arnoldi method belongs to a class of methods which can be interpreted as Krylov methods, either for an infinite-dimensional problem, or as a dynamically increasing companion linearization of an approximation of the problem [20–22]. This method is designed to find all eigenvalues close to a given shift, where the radius of convergence depends on properties of the matrix-valued function (2). Particularly, we adapt the variant with a tensor representation of the basis presented in [23], called the tensor infinite Arnoldi method (TIAR). For recent developments and problems see [24,25]. In this work we present a new computational approach to accurately approximate resonances of (1) efficiently, based on a high order Finite Element (FE) method combined with a specialization of TIAR.

More specifically, this paper contains the following new scientific contributions:

- We show that the eigenvalues of the operator function accumulate only at infinity.
- We obtain exponential convergence of the discretization error in the number of degrees of freedom by selecting enough number of DtN terms and then enhancing the polynomial order of the FE.
- We adapt TIAR for this problem class, and design an algorithm to efficiently compute the related quantities exploiting the structure of the NEP.
- We introduce a pole cancellation technique for meromorphic matrix-valued functions in order to maintain good performance for TIAR.
- We show that the algorithm is efficient with respect to CPU-time. In particular, the CPU-time is for large problems dominated by a precomputation of the LU-factorization
- We show that a higher order FE combined with TIAR is an efficient strategy for numerical approximation of resonances in exterior domains.

In Section 2 we introduce some background and preliminaries of problem (1), followed by a variational formulation, which is the base for the FE method in Section 3. In Section 4 we show how the spectral derivatives are computed, and how the algorithm is designed to exploit the particular structure of the NEP. Furthermore, in Section 4.4, we introduce a pole cancellation technique, which transforms the problem by removing poles in order to improve the convergence of TIAR. In Section 5, we perform numerical experiments for a known benchmark, and a more demanding test case in order to evaluate how the computational approach depends on the geometry. In Section 5, we provide a characterization of the performance of our approach. In particular, we show that the new infinite Arnoldi method together with a p-FE strategy is an efficient and reliable tool for resonance calculations with the DtN map.

2. Background and preliminaries

Results for the problem (1) can be found in a considerable amount of literature; see [3,26,27] and references therein. For $\operatorname{Im}\lambda > 0$ we have uniqueness results [26, Chapter VIII] and resonance values are therefore in the region $\operatorname{Im}\lambda < 0$.

Let $\Omega_a \subset \mathbb{R}^2$ be an open disk of radius a and boundary Γ_a. Assume $\eta \in L^\infty(\Omega_a)$ and that the non-negative function $\eta^2 - 1$ has compact support contained in Ω_a. A schematic setup of an example is illustrated in Fig. 1. The resonance problem restricted to Ω_a is formally to find non-trivial solutions (u, λ) such that (1) holds. The DtN operator on the circle Γ_a has the explicit form

$$\mathcal{G}(\lambda)u := \frac{1}{2\pi}\sum_{\nu=-\infty}^{\infty} g_\nu(\lambda)\, e^{i\nu\theta}\int_0^{2\pi} u(a,\theta')\, e^{-i\nu\theta'}\, d\theta', \tag{3}$$

where

$$g_\nu(\lambda) := \lambda\frac{H_\nu'(\lambda a)}{H_\nu(\lambda a)} \tag{4}$$

and $\mathcal{G}(\lambda) : H^{1/2}(\Gamma_a) \to H^{-1/2}(\Gamma_a)$ is bounded [3]. In the following, we identify the dual pairing $\langle\cdot,\cdot\rangle_{H^{-1/2}(\Gamma_a)\times H^{1/2}(\Gamma_a)}$ with the L^2-inner product $(\cdot,\cdot)_{\Gamma_a}$ over Γ_a. The theory presented in [3] can with minor changes be used in the present case to derive properties of a variational formulation of the problem.