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Rational eigenvalue problems and applications to photonic crystals

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ABSTRACT

We establish new analytic results for a general class of rational spectral problems. They arise e.g. in modelling photonic crystals whose capability to control the flow of light depends on specific features of the eigenvalues. Our results comprise a complete spectral analysis including variational principles and two-sided bounds for all eigenvalues, as well as numerical implementations. They apply to the eigenvalues between the poles where classical variational principles fail completely. In the application to multi-pole Lorentz models of permittivity functions we show, in particular, that our abstract two-sided eigenvalue estimates are optimal and we derive explicit bounds on the band gap above a Lorentz pole. A high order finite element method (FEM) is used to compute the two-sided bounds for a selection of eigenvalues for several concrete Lorentz models, e.g. polaritonic materials and multi-pole models.

1. Introduction

Many physical systems are passive in the sense that they do not produce energy, and materials are in general dispersive which, when frequency is the spectral parameter, leads to a non-linear spectral problem. Therefore a large number of systems are accurately described by Nevanlinna functions (sometimes also called Herglotz functions) whose values are differential operators. In systems theory operator-valued Nevanlinna functions arise as transfer functions and have been studied intensively [8,7,3]; in spectral theory, they arise as Schur complements and have been known as versatile tools to study operator matrices [46]. However, we still lack a more detailed understanding of a class of rational Nevanlinna operator functions that are sufficiently general to cover some important physical applications, such as acoustic and electromagnetic

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problems with frequency dependent materials e.g. in photonic crystals. While applied research on the latter is progressing rapidly, mathematical research in this direction has started, but is still in its infancy [15,14,43].

Our aim is to establish a comprehensive picture of the spectral properties for such rational operator functions under weak assumptions. The novelty of our approach is that it applies, in the case of several poles, to the eigenvalues between the poles where classical min-max variational principles fail completely. As a result, in applications to photonics, we cover piecewise constant multi-pole Lorentz models [27,41]

$$\epsilon(\cdot,\omega)=\sum_{m=1}^{M}\epsilon_m(\omega)\chi_{\Omega_m}(\cdot),\quad \epsilon_m(\omega)=\epsilon_{m,\infty}+\epsilon_{m,\infty}\sum_{\ell=1}^{L_m}\frac{\omega_{p,m,\ell}^2}{\omega_{0,m,\ell}^2-\omega^2}, \tag{1.1}$$

periodic on some bounded domain $\Omega=\Omega_1\cup\cdots\cup\Omega_M$, as well as permittivity functions $\epsilon(\cdot,\omega)$ where the linear part of the corresponding operator function has eigenvalues $\lambda:=\omega^2$ below the Lorentz poles $\omega_{p,m,\ell}^2$. The abstract operator functions we consider are meromorphic on the complex plane and have a finite number of poles which are real (including ∞) and of first order. Moreover, multiplied by -1, they have the Nevanlinna property in the sense that the values on the real axis are self-adjoint operators, the residues are non-positive, and the derivatives are non-negative between the poles. This property enables us to introduce generalized Rayleigh functionals, to establish variational principles, and to derive two-sided estimates for *all* eigenvalues of this class of rational operator functions. Since our results cover both infinite and finite dimensional problems, they apply to the original problem as well as to the numerical approximation. This allows us e.g. to establish dimension conditions ensuring that FEM computations reproduce the possible index shift in the variational principle correctly.

We demonstrate the efficacy of the new theory for unbounded operator functions that arise in modelling photonic crystals. These dielectric nano-structured materials which are used to control and manipulate the flow of light [24] are commonly modelled by periodic Lorentz permittivity functions (1.1) with several rational terms. Examples show that our abstract two-sided eigenvalue estimates are sharp, and we derive explicit bounds on the band gap above a Lorentz pole. The operator function is discretised with a high order finite element method and several concrete examples e.g. for polaritonic materials illustrate the general theory. In particular, we compute the two-sided estimates of a selection of eigenvalues and we illustrate the accumulation of eigenvalues at the poles and the corresponding singular sequence. In most examples a continuous finite element method is used to compute the eigenvalues, but in cases were a block diagonal mass matrix is an advantage a discontinuous Galerkin method is employed.

The paper is organized as follows. In Section 2 we set up the required operator theoretic framework. In Section 3 we consider the one pole case and establish min-max variational characterizations and two-sided estimates for all eigenvalues. In Section 4 we generalize the min-max principles to the multi-pole case and identify cases where a band gap occurs. In Section 5 we apply our abstract results to photonic crystals with multi-pole Lorentz models (1.1). Section 6 contains the numerical finite element analysis for several material models, illustrating different features of the abstract results such as the occurrence of an index shift or band gaps.

Throughout this paper we use the following notations and conventions. All Hilbert spaces are separable. For a closed linear operator T in a Hilbert space $\mathcal{H}$ we denote by $\ker T$, $\operatorname{ran} T$, $\rho(T)$, $\sigma(T)$, and $\sigma_{\mathrm{p}}(T)$ its kernel, range, resolvent set, spectrum, and point spectrum, respectively; the essential spectrum of T is defined as $\sigma_{\mathrm{ess}}(T):=\{\lambda\in\mathbb{C}: T-\lambda \text{ is not Fredholm}\}$. If T is self-adjoint, then $\lambda\in\sigma_{\mathrm{ess}}(T)$ iff $\lambda\in\sigma(T)$ and λ is *not* an isolated eigenvalue of finite multiplicity. Further, for a Borel set $I\subset\mathbb{R}$, we denote by $\mathcal{L}_I(T)$ the spectral subspace of T corresponding to the set I and, if T is bounded from below and $\mu<\min\sigma_{\mathrm{ess}}(T)$, by $N(T,\mu):=\dim\mathcal{L}_{(-\infty,\mu]}(T)$ the number of eigenvalues of T that are $\le\mu$ counted with multiplicities.