Efficient Photonic Component Analysis via AAA Rational Approximation

Lin Zschiedrich
JCMwave GmbH, Berlin, Germany
https://orcid.org/0000-0002-1969-0633

Fridtjof Betz
Zuse Institute Berlin, Germany
https://orcid.org/0000-0003-2193-7188

Felix Binkowski
Zuse Institute Berlin, Germany
JCMwave GmbH, Berlin Germany
https://orcid.org/0000-0002-4728-8887

Lilli Kuen
Weierstrass Institute Berlin, Germany
https://orcid.org/0000-0002-3183-4222

Martin Hammerschmidt
JCMwave GmbH, Berlin, Germany
https://orcid.org/0000-0003-0291-1599

Sven Burger
Zuse-Institute, Berlin
JCMwave GmbH, Berlin Germany
https://orcid.org/0000-0002-3140-5380

***Abstract*—We review the application of the AAA algorithm for rational approximation of the optical response function in photonic devices. Originally developed to efficiently interpolate sampled response data, the AAA algorithm also enables the accurate and stable computation of resonances, e.g., quasinormal modes (QNMs), along with their corresponding field distributions. Our approach applies to general nonlinear eigenproblems and can handle branch cuts without introducing spurious or artificial modes. It can further be applied to analyze VCSEL systems and photonic waveguides.**

***Index Terms*—Photonic modes, rational approximation, AAA algorithm, quasinormal modes (QNM), nonlinear eigenvalue problems, resonance analysis, optical response, VCSEL.**

I. Problem Setup

We consider time-harmonic light scattering problems as described by the second-order Maxwell's equation

$$\nabla \times \mu^{-1} \nabla \times \mathbf{E} - \omega^2 \epsilon \mathbf{E} = i\omega \mathbf{J}, \tag{1}$$

where $\mathbf{E}(\mathbf{r}, \omega) \in \mathbb{C}^3$ is the scattered electric field and $\omega \in \mathbb{C}$ is the angular frequency. The source is modeled as an electric current density $\mathbf{J}(\mathbf{r}) \in \mathbb{C}^3$. The material properties are integrated into the model through the permittivity $\epsilon(\mathbf{r}, \omega)$ and permeability $\mu(\mathbf{r}, \omega)$ tensors, and $\mathbf{r} \in \mathbb{R}^3$ is the position. Light scattering problems with an extended illumination such as a plane wave can be transformed in the above form (1). Furthermore, Maxwell's equation (1) is supplemented with a radiation condition, realized by perfectly matched layers (PMLs), and/or periodic boundary conditions which may also depend nonlinearly on ω.

In this work, we review the recently introduced approaches from Refs. [1]–[4] based on the AAA algorithm [5]. To analyze or to optimize the optical system, a measurable quantity of interest $f(\omega)$ (response function) is extracted from the electromagnetic field such as far-field amplitudes, Purcell factors, coupling coefficients, etc. As our framework relies on the meromorphic nature of the response $f(\omega)$, special care is needed for quadratic quantities to circumvent complex conjugation; see [6]. From the perspective of this work, the numerical solver for Maxwell's equation (1) is a complete black box. We want to characterize the system only from the knowledge of the response function $f(\omega)$ at discrete sampling points (ω_k, f_k) [5]. The efficiency of the algorithm corresponds to the number of required sampling points to reach a desired accuracy.

This is in contrast to a traditional QNM computation [7], [8] with an eigensolver such as Arpack [9]. An algebraic eigensolver relies on the application of the system matrices together with their sparse inversion and needs adaptions to cope with the nonlinearity of the material tensors or the boundary conditions [10]. The advantage of our approach is that the excitation source as well as the relevant quantity of interest are included in the analysis step, so that the framework is considered as *physically driven*. We can prioritize the computed modes by their impact on the quantity of interest and how strongly they are excited by the given source. In this way, an intrinsic mode selectivity allows to easily filter out non-physical modes which may be caused by the truncation of the PML system.

II. AAA Rational approximation

The **A**daptive **A**ntoulas–**A**nderson (AAA) algorithm [5] gives an approximation of a scalar-valued function $f(\omega)$ by a rational function $r(\omega)$ in a barycentric representation. A number M of freely selectable sampling points $\omega_k \in Z \subseteq \mathbb{C}$ and corresponding function values $f_k = f(\omega_k)$ are the input for the algorithm. The algorithm greedily adds sampling points $\hat{\omega}_j$ to a subset $\hat{Z} \subset Z$, together with the corresponding function values $\hat{f}_j$ until reaching the demanded accuracy. Then, each iteration within the algorithm leads to a rational approximation $r(z)$ of order $m-1$,

$$r(\omega) = \frac{n(\omega)}{d(\omega)} = \sum_{j=1}^{m} \frac{\hat{w}_j \hat{f}_j}{\omega - \hat{\omega}_j} \Bigg/ \sum_{j=1}^{m} \frac{\hat{w}_j}{\omega - \hat{\omega}_j}\ , \tag{2}$$

where the weights $\hat{w}_j$ minimize the error

$$\sum_{\omega_k \in Z \setminus \hat{Z}} |f_k\, d(\omega_k) - n(\omega_k)|^2. \tag{3}$$

The barycentric representation of the $r(\omega)$ forms the foundation of the AAA algorithm and enables the efficient computation of the rational approximation. It has removable singularities at $\hat{z}_j \in \hat{Z}$ and the limit $\lim_{z\to\hat{z}_j} r(z) = \hat{f}_j$ exists. Therefore, the approximation $r(z)$ interpolates the function values $\hat{f}_j$. The zeros of $n(z)$ and $d(z)$ are the zeros and poles of $r(z)$, respectively. They are provided as the eigenvalues of generalized eigenproblems. The residues of the approximative response function $r(\omega)$ are considered as the *modal contributions* of the corresponding poles.

III. Applications

Characterization of chiral metaurfaces, sensitivity analysis

In [1], we characterized a chiral metasurface by its modal contributions. As a surplus of the AAA algorithm, the sensitivities on the geometrical parameters can be easily computed just from derivative data of the response function. Furthermore, the AAA algorithm is exploited to directly solve the eigenproblems, i.e., we show how to superimpose the field values at the sampling points to form an approximation of the QNM field, which is scaled according to its excitation by the chosen source.

Finding relevant VCSEL resonance modes

This example is taken from [2], where we applied the Riesz contour integral method [11] to compute the fundamental mode of a vertical-cavity surface-emitting laser (VCSEL). We fare much better with the new AAA based approach. The following table gives the convergence of the fundamental mode eigenvalue with the number of sampling points that were equidistantly chosen within the wavelength interval $[986\mathrm{nm}, 976\mathrm{nm}]$.

$\#n$	$\Re(\lambda)[\mathrm{nm}]$	$\Im(\lambda)[\mathrm{nm}]$	rel. err
2	9.8107e+02	0.0000e+00	1.48e-03
3	9.7919e+02	2.9976e+00	2.89e-03
5	9.7936e+02	1.5045e+00	1.36e-03
9	9.7965e+02	1.9669e-01	2.46e-05
17	9.7963e+02	2.0128e-01	5.99e-07
33	9.7963e+02	2.0121e-01	2.29e-08
65	9.7963e+02	2.0120e-01	1.29e-08
81	9.7963e+02	2.0122e-01	4.49e-09

TABLE I: Convergence of the fundamental mode eigenvalue with the number of equidistant sampling points on the real axis. Five sampling points are needed to observe convergence. The saturation from 33 sample points onwards is due to the numerical condition of the FEM system.

Dealing with branch cuts

In [3], we applied the AAA algorithm to a periodic scattering problem where the response function exhibits branch cuts due to vanishing diffraction orders. When sampling along the real frequency axis, these branch cuts manifest as clusters of poles, complicating the analysis. This issue can be resolved using a complex coordinate transformation that maps the frequency plane onto a Riemann surface without branch cuts. This transformation reveals resonance modes that would otherwise be obscured, thereby clarifying the underlying physical mechanisms.

Waveguide analysis

For waveguide problems, the optical response is preferable considered as dependent on the propagation constant k_z. Our framework also applies to that case; see [4]. For many practical applications involving photonic cyrstal fibers, the fundamental mode is embedded in a cluster of cladding modes which renders eigenvalue computations costly and requires to filter out the relevant mode. Here, our framework allows to choose a source term located in the core region of the fiber which only weakly excites the cladding modes.

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