

# A Framework to Compute Resonances Arising from Multiple Scattering

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Numerous natural and technological phenomena are governed by resonances. In nanophotonics, resonances often result from the interaction of several optical elements. Controlling these resonances is an excellent opportunity to provide light with properties on demand for applications ranging from sensing to quantum technologies. The inverse design of large, distributed resonators, however, is typically challenged by high computational costs when discretizing the entire system in space. Here, this limitation is overcome by harnessing prior knowledge about the individual scatterers that form the resonator and their interaction. In particular, a transition matrix multi-scattering framework is coupled with the state-of-the-art adaptive Antoulas–Anderson (AAA) algorithm to identify complex poles of the optical response function. A sample refinement strategy suitable for accurately locating a large number of poles is introduced. The AAA algorithm is tied into an automatic differentiation framework to efficiently differentiate multi-scattering resonance calculations. The resulting resonance solver allows for efficient gradient-based optimization, demonstrated here by the inverse design of an integrated exciton-polariton cavity. This contribution serves as an important step towards efficient resonance calculations in a variety of multi-scattering scenarios, such as inclusions in stratified media, periodic lattices, and scatterers with arbitrary shapes.

nanophotonic systems to obtain desired properties for specific applications. For example, they can promote and shape the emission of dipolar (quantum) emitters<sup>[1–3]</sup> and lasers.<sup>[4,5]</sup> They are fundamental to various wavelength-selective devices like multiplexers and all-pass filters.<sup>[6]</sup> The interplay among multiple resonances can lead to the emergence of complex behavior in observable quantities,<sup>[7]</sup> including Fano resonances<sup>[8]</sup> and the optical Vernier effect.<sup>[9]</sup>

The interaction between coupled resonators can create a rich resonance spectrum beyond the original resonances of the uncoupled building blocks. By altering the shape and arrangement of subcells of such composite resonators, their spectrum can be tailored on demand. As a result, composite resonators play an enabling role in various fields of science and technology, including photonic crystal cavities, e.g., as interfaces for quantum computing,<sup>[3,10]</sup> coupled-resonator optical waveguides<sup>[11]</sup> for broadband but sharp integrated optical filters,<sup>[12]</sup> high contrast grating cavities for silicon integrated lasers,<sup>[4]</sup> and

all-optical polariton transistors.<sup>[13]</sup> Similarly, resonant metamaterials formed by regular arrangements of subcells are of current interest.<sup>[14–16]</sup> As such, they find applications as mirrors in, e.g., macroscopic Fabry–Perot resonators.<sup>[17]</sup>

## 1. Introduction

Resonances play an integral role in many photonic applications. Deliberately tailored resonances can force the light in

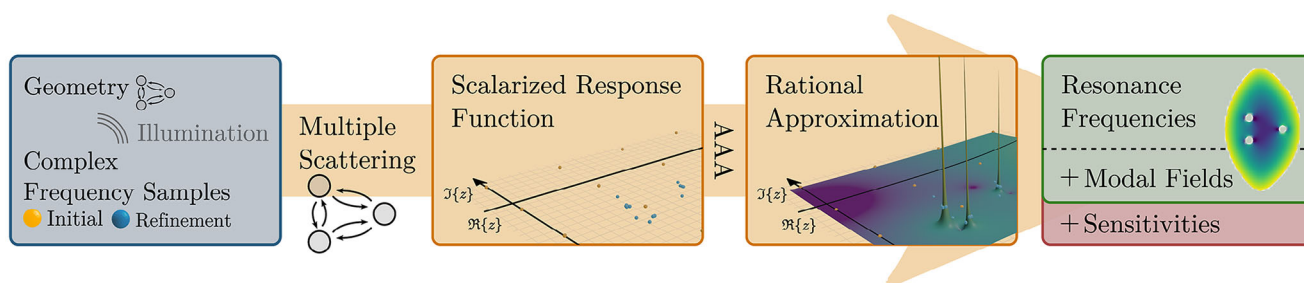
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**Figure 1.** Schematic representation of the workflow of our proposed method: Single scatterers are arranged to form a resonator. The optical response is efficiently evaluated by multiple-scattering simulations at complex frequency samples  $z_k$ . A scalarized response function  $f(z_k)$  is computed from the simulated optical response. Then, the AAA algorithm is used to construct a rational approximation from the samples in the complex frequency plane. While the resonance frequencies can be directly obtained from the resulting approximation, a single additional scattering simulation is performed to obtain the corresponding modal fields. Moreover, the sensitivities of the resonance frequencies and their contribution to observable quantities (expressed in terms of its residue) w.r.t. any degree of freedom characterizing the system can be obtained thanks to the automatic differentiation of the computational workflow. As a consequence, we can subject the resonances to the inverse design of the composite resonator (not shown).

Electromagnetic resonances are known by many names across the literature, including quasi-normal modes, resonant states, natural modes, decaying states, and leaky modes. They are solutions to the time-harmonic source-free Maxwell equations obeying radiative boundary conditions. In passive systems with radiative and/or material losses, this eigenproblem is non-Hermitian. This results in complex-valued resonance frequencies  $\tilde{z}$ , with a negative imaginary part (in the sign convention at hand), which corresponds to the resonances' decay rate. The non-Hermitian character challenges the normalization of the modal fields that diverge away from the resonator. Various normalization strategies addressing this field divergence have been extensively debated. For the sake of brevity, we refer the interested reader to the following collection of recent articles.<sup>[18–24]</sup>

Accurately and efficiently determining the resonances in complex photonic systems is an ongoing research challenge.<sup>[25]</sup> Proposed strategies include the harmonic inversion of time-domain simulations,<sup>[26,27]</sup> perturbative methods<sup>[28]</sup> such as the so-called resonant state expansion,<sup>[29,30]</sup> and the use of Fredholm-type integral equations.<sup>[26,31]</sup> Nevertheless, most state-of-the-art methods for computing electromagnetic resonances follow one of two distinct approaches. The first approach directly treats the nonlinear eigenproblem (NEP) posed by the source-free Maxwell equations in dispersive media. This approach most commonly relies on some finite-element discretization paired with schemes to linearize the NEP.<sup>[32,33]</sup>

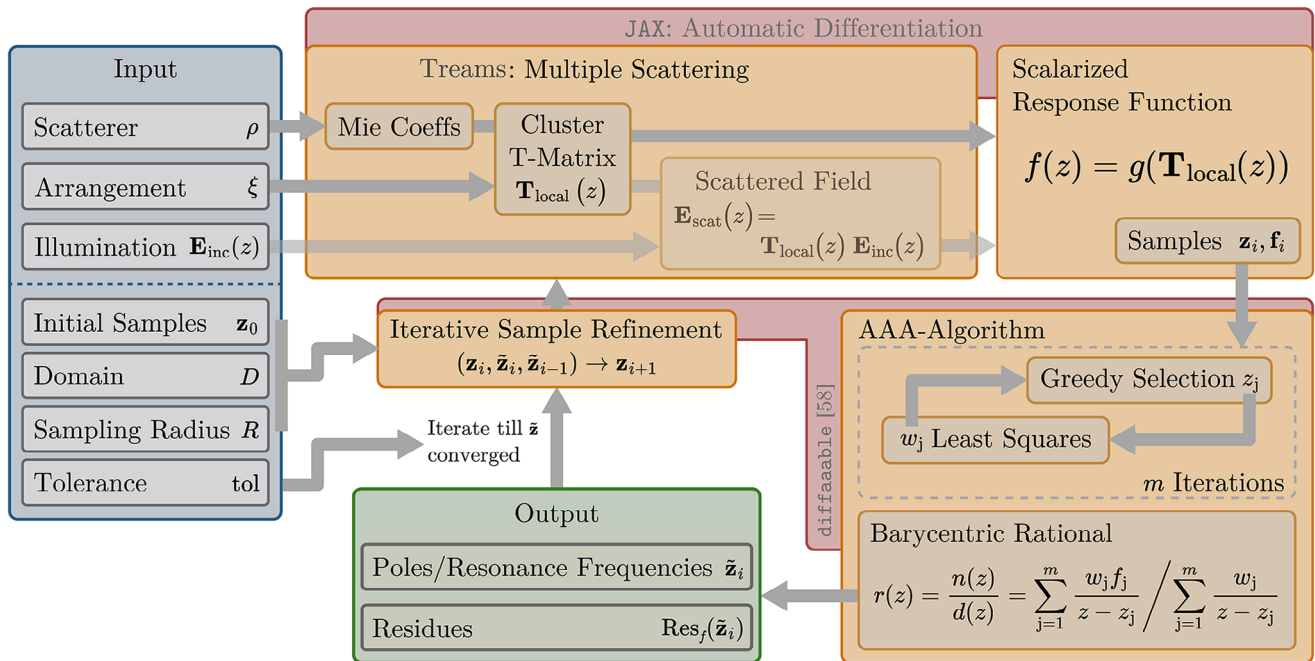
In a second approach, the resonances can be found by considering a related inhomogeneous problem, where auxiliary sources are introduced into the system. This scattering problem will be formalized in Section 2.1. Crucially, its analytic continuation has singularities at complex frequencies that correspond directly to the resonances of the original system. These singularities can be searched for via a variety of methods, e.g., gradient descent<sup>[34]</sup> and contour integration (with the Cauchy residue theorem).<sup>[35,36]</sup>

Owing to the fixed excitation frequency, this approach conveniently allows us to use any solver capable of evaluating the scattering problem at complex frequencies. Thus, it enables the use of further efficient problem-specific evaluation strategies, like the boundary element method,<sup>[34,37,38]</sup> or the Fourier modal

method.<sup>[39–41]</sup> When treating the entire resonator as a single large system, one challenge pertinent to both approaches are the different length scales involved in many relevant compound resonators. Such treatment requires extensive memory and computing power. However, it is not necessary to consider the entire space occupied by a given photonic resonator when it is composed of multiple individual elements.<sup>[35,42,43]</sup>

Here, we instead address the subcells individually and *a-posteriori* include their mutual coupling. **Figure 1** indicates schematically how we combine established methods for multiple-scattering resonance calculations. Specifically, we use analytical expressions for the electromagnetic wave propagation in a homogeneous background medium via the transition matrix formalism (TMF).<sup>[35,44]</sup> To minimize the number of function evaluations while robustly recovering all relevant resonances, we choose the AAA algorithm<sup>[45]</sup> for pole finding.<sup>[46]</sup> In contrast to contour integration methods, it allows us to freely add and remove frequency samples, thus supporting fine-grain adaptive refinement strategies, which is crucial to efficiently determining the rich resonance spectra of large ensembles of scatterers.

Additionally, we combine the established derivatives within the AAA algorithm<sup>[46]</sup> with automatic differentiation<sup>[47]</sup> of the TMF to obtain gradients of the resonance frequencies. Having these gradients at hand, we demonstrate the inverse design of resonances for a cavity of contemporary interest.<sup>[13]</sup> We demonstrate how to optimize the quality factor of a selected mode, achieving a level where it only remains limited by nonradiative losses. The considered system is an integrated cavity defined by dielectric posts in a stratified medium, arranged sequentially to form two mirrors. The stratified medium contains the ladder-type polymer MeLPPP that supports room-temperature exciton-polaritons.<sup>[48]</sup> These quasiparticles, which arise from the coupling of photons and excitons, form in the strong light-matter interaction regime when the polymer is placed in a wavelength-scale optical microcavity with a sufficiently high quality factor. These exciton-polariton devices have the potential to become crucial components of integrated all-optical computing platforms. To develop sophisticated polaritonic circuits and systems, it is essential to *in-silico* optimize individual cavities and arrangements of coupled cavities.



**Figure 2.** Flowchart detailing the procedure to determine resonance frequencies of a given arrangement  $\xi$  of scatterers. The scattering problem is solved for an initial set of samples  $\mathbf{z}_0$ . The solutions are scalarized as chosen by the user (via the choice of  $g(\mathbf{T}_{\text{local}})$ ). The sample pairs are aggregated into the vectors  $\mathbf{z}_i$  and  $\mathbf{f}_i$ . The AAA algorithm is then used to estimate the pole positions  $\bar{\mathbf{z}}_0$ , equivalent to the complex resonance frequencies. To ensure the accuracy of these resonance frequencies, samples are iteratively added in the vicinity of poles, which are selected according to Algorithm ISR. User inputs are indicated in the blue box to the left. Methods to calculate sensitivities of the resonances (indicated in red) are further discussed in Section 3.4.

## 2. Experimental Section

In the following, a detailed description of the proposed computational workflow will be provided. **Figure 2** guides the reader through the approach, starting with the central multiple-scattering formalism and continuing clockwise.

### 2.1. The Scattering Problem: Transition Matrix Formalism

Instead of directly treating the NEP, the second approach mentioned in the introduction was taken and the resonances were identified as singularities of the time-harmonic Maxwell equations including sources:<sup>[36]</sup>

$$\nabla \times \mu^{-1}(\mathbf{r}, z) \nabla \times \mathbf{E}(\mathbf{r}, z) - z^2 \varepsilon(\mathbf{r}, z) \mathbf{E}(\mathbf{r}, z) = iz \mathbf{J}(\mathbf{r}, z). \quad (1)$$

Here,  $\mathbf{E}(\mathbf{r}, z)$  is the position dependent total electric field resulting from the excitation by the source current  $\mathbf{J}(\mathbf{r}, z)$  at the complex frequency  $z$ , in and around the entire resonator. The  $e^{-izt}$  sign convention is used in this contribution.

Let us consider a resonator consisting of an ensemble of individual optical elements (denoted as scatterers) embedded in a homogeneous background. With all sources located outside the individual scatterers, their individual response can be described in terms of the scattered field  $\mathbf{E}_{\text{scat}}$  resulting from some incident field  $\mathbf{E}_{\text{inc}}$  [18], Annex 2]. The incident and scattered fields can be expanded into a set of basis functions that are elementary solutions to Maxwell's equations in the background medium. The vector cylindrical waves (VCW; 2D) and vector spherical waves

(VSW; 3D) each form a complete basis of such solutions. By expressing the incident and scattered field at a complex frequency  $z$  as coefficient vectors in such a basis, the scattering response from an individual scatterer can be encapsulated into the operator  $\mathbf{T}(z)$  defined by:

$$\mathbf{p}(z) = \mathbf{T}(z) \mathbf{a}(z), \quad (2)$$

where  $\mathbf{a}(z)$  are the incident field coefficients and  $\mathbf{p}(z)$  are the scattered field coefficients. To make the expressions numerically tractable, the multipolar basis of  $\mathbf{a}(z)$  and  $\mathbf{p}(z)$  is typically truncated by a maximum multipolar order  $m_{\text{max}}$  (2D) or degree  $l_{\text{max}}$  (3D). Truncating the multipolar order permits the expression of  $\mathbf{T}(z)$  as a finite matrix. The error introduced by the truncation is discussed in Section S3 (Supporting Information). Determining  $\mathbf{T}(z)$  is at the core of solving the scattering problem for a single scatterer. A variety of methods to numerically evaluate  $\mathbf{T}(z)$  for arbitrarily shaped scatterers exist.<sup>[49–51]</sup> Analytical expressions for  $\mathbf{T}(z)$  are available for high-symmetry scatterers, such as infinitely extended cylinders (circles in 2D) and spheres.<sup>[52]</sup> These are commonly referred to as (generalized) Mie coefficients (first block of “Multiple Scattering” in Figure 2). As shown in the Section S1.1 (Supporting Information), the Mie coefficients can be evaluated at complex frequencies  $z$  and are meromorphic with respect to  $z$  in the relevant section of the complex plane.

By considering the scattered field of one scatterer as part of the incident field to all other scatterers arranged to form the resonator, and vice versa, one can fully describe the effect

of multiple scattering in a cluster (central block of “Multiple Scattering” in Figure 2):<sup>[44]</sup>

$$\mathbf{p}_{\text{local}}(z) = \underbrace{[1 - \mathbf{T}_{\text{diag}}(z)\mathbf{C}^{(3)}(z)]^{-1}\mathbf{T}_{\text{diag}}(z)}_{\mathbf{T}_{\text{local}}(z)} \mathbf{a}_{\text{local}}(z). \quad (3)$$

Here,  $\mathbf{T}_{\text{diag}}(z)$  is the block diagonal matrix constructed from the  $\mathbf{T}(z)$  for each isolated constituent scatterer.  $\mathbf{C}^{(3)}(z)$  encapsulates the translation coefficients to transform the scattered field from one scatterer into the basis of the other scatterers. It was noted that  $\mathbf{C}^{(3)}(z)$  is holomorphic in  $z$  in the relevant domain (Section S1.2, Supporting Information). The field coefficients and the total transition matrix in Equation (3) are expressed in the joint local basis of the constituent particles, containing VSWs/VCWs around all scatterers. A basis change to a global basis with VSWs/VCWs around a single shared origin is possible.

The collective response of the cluster to every possible excitation is encapsulated in the resulting  $\mathbf{T}_{\text{local}}$ -matrix. As a consequence,  $\mathbf{T}_{\text{local}}(z)$  contains all resonances that interact with the environment as poles of its entries. The fact that the transition matrix, and equivalently the scattering matrix  $\mathbf{S} = \mathbf{1} + 2\mathbf{T}$ ,<sup>[53]</sup> contain the resonances of the object they describe is well established.<sup>[54–57]</sup> The  $\mathbf{T}$ -matrix permits various scalarization strategies to arrive at a scalar meromorphic response function  $f(z)$ , later used for pole finding. This choice determines the residues, which can help to emphasize poles of interest. Contrary to the scattering problem in terms of a source current  $J(\mathbf{r}, z)$ , within the  $\mathbf{T}$ -matrix formalism it is optional to select a source (indicated by the translucent third block of “Multiple Scattering” in Figure 2, also see Section 3.3 for possible benefits). Alternatively, the transition matrix, which already contains the response to all possible excitations, can be scalarized by some linear function  $g(\mathbf{T}_{\text{local}}(z))$ , for example, linear combinations of selected entries or the determinant of  $\mathbf{T}_{\text{local}}(z)$ .

## 2.2. Complex Pole Finding: AAA Rational Approximation

With this strategy to efficiently evaluate the scalarized response function  $f(z)$  in place, it remains to identify its poles. In principle, any of the aforementioned pole-finding methods could be applied. The recently published AAA algorithm was used for rational approximation<sup>[45,46]</sup> due to its multiple benefits:

1. It is less dependent on *initial values* to identify all relevant poles. Methods based on gradient descent particularly suffer from this limitation.
2. It provides excellent *convergence* with the number of frequency samples.
3. The convergence characteristics are complemented by the freedom to add and remove samples. As such, it permits *refinement strategies* to iteratively add a small number of samples around relevant poles (see Algorithm ISR). This feature distinguishes the approach from contour integral methods, as numerical quadratures require specific sampling strategies for a comparable convergence.

**Algorithm ISR** Algorithm to reduce the number of function evaluations needed for convergence of the poles estimated via the AAA approximation. Starting from a vector of initial samples  $\mathbf{z}_0$  a first AAA approximation is constructed and the corresponding poles  $\bar{\mathbf{z}}$  are determined. In the first iteration, one additional sample per estimated pole is placed in the pole’s vicinity (at a fixed distance  $R$  and random direction  $\varphi_{\text{rand}}$  from the pole) if it lies within the domain of interest  $\mathcal{D}$ . In successive iterations, additional samples are only placed if the corresponding pole is not matched by any pole in the previous iteration (within some specified tolerance), i.e., the pole’s position has not yet converged. The algorithm terminates after all poles have converged.  $l$  is the iteration number.  $\mathbf{z}_l$ ,  $\mathbf{f}_l$ , and  $\bar{\mathbf{z}}_l$  are vectors containing the frequency samples, corresponding function values, and estimated poles, respectively.  $\mathbf{z}_{-1}$ ,  $\mathbf{f}_{-1}$ , and  $\bar{\mathbf{z}}_{-1}$  are empty. The  $\oplus$  symbol indicates the concatenation of vectors.

Algorithm ISR Iterative Sample Refinement

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 $\mathbf{z}_{\text{add}} \leftarrow \mathbf{z}_0$ 
While  $\mathbf{z}_{\text{add}}$  not empty do
     $\mathbf{z}_l \leftarrow \mathbf{z}_{l-1} \oplus \mathbf{z}_{\text{add}}$ 
     $\mathbf{f}_l \leftarrow \mathbf{f}_{l-1} \oplus [f(z) \text{ for } z \in \mathbf{z}_{\text{add}}]$ 
     $\bar{\mathbf{z}}_l \leftarrow \text{AAA}(\mathbf{z}_l, \mathbf{f}_l)$ 
     $\mathbf{z}_{\text{add}} \leftarrow [\bar{\mathbf{z}} + R e^{i\varphi_{\text{rand}}} \text{ for } \bar{\mathbf{z}} \in \bar{\mathbf{z}}_l \cap \mathcal{D}$ 
        if  $\min|\bar{\mathbf{z}} - \bar{\mathbf{z}}_{l-1}| > \text{tol}]$ 
     $l \leftarrow l + 1$ 
end while

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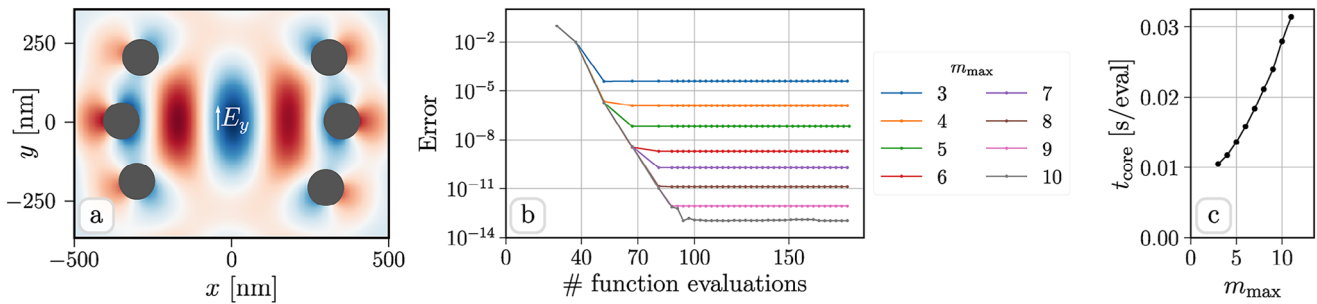
The barycentric rational form is at the heart of the AAA algorithm:

$$r(z) = \frac{n(z)}{d(z)} = \sum_{j=1}^m \frac{w_j f_j}{z - z_j} \bigg/ \sum_{j=1}^m \frac{w_j}{z - z_j} \approx f(z). \quad (4)$$

It possesses the interpolation property of reproducing  $\lim_{z \rightarrow z_j} r(z) = f_j$ . Using this property, the approximation is iteratively constructed by greedily aggregating a selection of considered samples  $z_j$  from the set of all samples (with elements  $z_k$ ). In every step, the corresponding weights  $w_j$  are chosen to minimize the residual error at the remaining samples (schematically indicated in “AAA-Algorithm” in Figure 2). The poles and their residues are easily accessible from the constructed approximation (see “Output” in Figure 2). However, they might not yet have the desired accuracy at this point.

The third property of the AAA algorithm mentioned above allows us to freely place additional samples near estimated poles to refine them.<sup>[46]</sup> Here, this idea was generalized to an iterative aggregation scheme for  $z_k$  (see Algorithm ISR indicated in Figure 2 by “Adaptive Refinement”). This modification allows us to efficiently and simultaneously find a *large* number of relevant poles (see Section 3.3). It avoids overly refining poles that have already been localized to a satisfactory degree.

As discussed in ref. [46], the samples not incorporated in  $r(z)$  can be used to find the *derivatives* of  $w_j$  w.r.t. the sampled values  $\mathbf{f}$ . A Python implementation of the derivatives compatible with JAX automatic differentiation is provided with this contribution<sup>[58]</sup> (represented by the lower red box in Figure 2). In conjunction with the automatically differentiable TMF (represented by the upper red box in Figure 2), this allows us to compute the gradients of the poles (i.e., resonance frequencies) relative to all degrees of freedom in the design. This ability is



**Figure 3.** Convergence study of the proposed method for a small resonator made from an assembly of cylindrical scatterers. Thirteen resonances between 1.6 and 2.7 eV are considered simultaneously a) Dominant field component of the resonance with the lowest losses located at  $\tilde{z} \approx (2.142 - 0.074i)$  eV. The field is not evaluated inside the cylindrical scatterers, where the expansion of the scattered field into radiating VCWs is not valid. b) Execution time on a single core per function evaluation depending on the truncation order  $m_{\max}$  of the cylinders' T-matrix. c) Convergence of the error in resonance frequencies with an increasing number of frequency samples, given as the maximum relative error (here denoted as "Error") of the relevant poles compared to reference poles evaluated with  $m_{\max} = 11$ . To clearly show the convergence behavior, the samples were selected by Algorithm ISR modified to yield at least three new samples (close to the most volatile poles) for 38 iterations.

key to performing gradient-based inverse design as described in Section 3.4. Implementation details for the AAA derivatives are laid out in Section S2 (Supporting Information).

### 3. Results

Due to their strong and ultrafast nonlinearity, exciton-polaritons hold great potential as a platform for all-optical logic operations. However, chip integration is required to scale up and leverage their ultra-fast switching in complex circuits. Ongoing efforts use cavities formed by high contrast grating (HCG) meta-mirrors for this purpose.<sup>[13]</sup> These cavities are fabricated in an SOI platform by nanostructuring the top-silicon layer, which is optically isolated from the silicon substrate by a buried oxide layer. The organic ladder-polymer MeLPPP is spin-coated onto the cavity and encapsulated by a layer of  $\text{Al}_2\text{O}_3$  deposited by atomic layer deposition (see Figure 5a). As the encapsulated polymer has a higher refractive index than the  $\text{SiO}_2$  below and the air above, it supports vertically confined slab modes. Lateral photonic confinement is realized by the lithographically defined silicon nanopillars.

The examples we will treat throughout the rest of this contribution are chosen to showcase selected aspects of the proposed method, while introducing relevant concepts, later used in the inverse design of such integrated polariton cavities. We start by examining the computational cost and convergence of finding the resonance frequencies for a small number of coupled scatterers. We then demonstrate how modal fields can be evaluated and go over methods for emphasizing or suppressing resonances using an appropriate choice of excitation. In particular, we study a macroscopic cavity formed by metamaterial mirrors, robustly recovering its rich spectrum and modal fields. Tracking relevant modes becomes particularly important when using the available sensitivities for gradient-based inverse design, which is discussed last.

#### 3.1. Resonance Frequencies

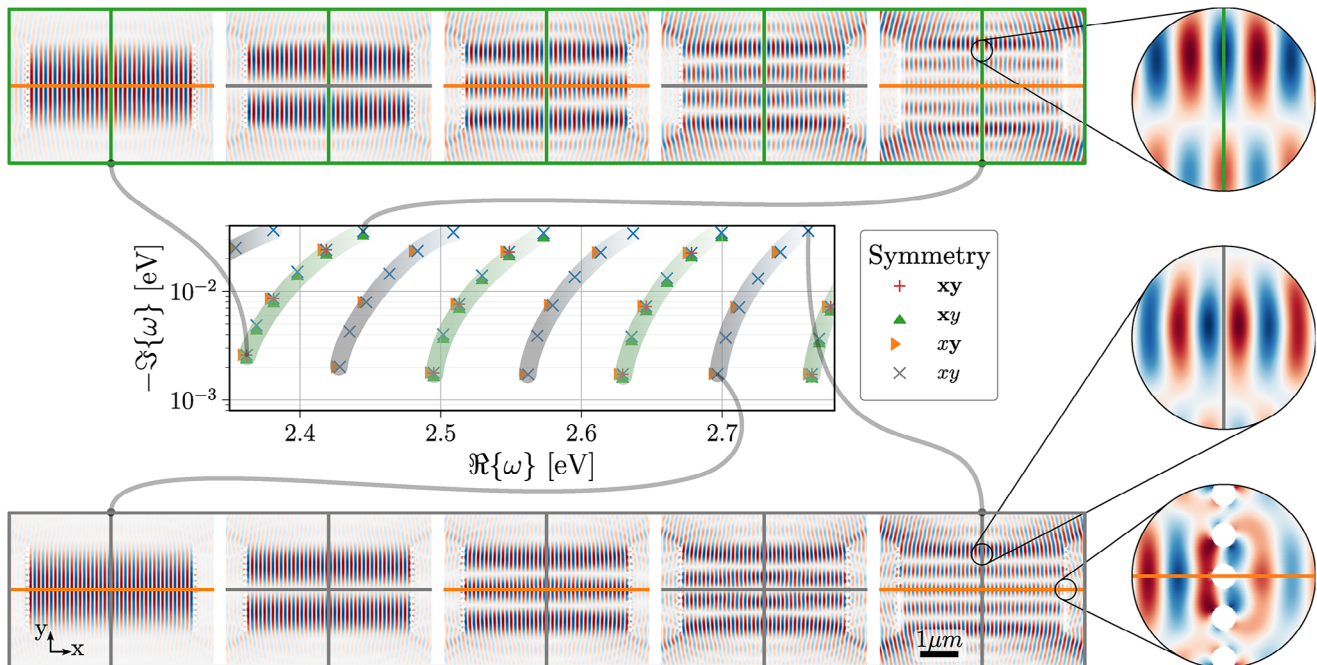
Let's consider the first example resonator made of 6 dispersive silicon pillars (the parameters of the Lorentz oscillator model are provided in Section S4, Supporting Information) embedded in a background permittivity  $\epsilon_{r,\text{bg}} = 2.9 + 0.001i$  as shown

in Figure 3a. The pillars have a radius of  $R = 55$  nm and are positioned such that the center-to-center distance of the central cylinders is 700 nm. The upper and lower posts are displaced by 200 nm in the y-direction and 50 nm inwards along the x-direction. Light is scattered between the cylinders leading to the formation of collective resonances. Figure 3a illustrates the electric field distribution of one such resonance with frequency  $\tilde{z} \approx (2.142 - 0.074i)$  eV. In the following, we will analyze the accuracy and computational cost of determining multiple resonance frequencies simultaneously using our method.

Figure 3b shows how the error of the resonance frequencies converges while adaptively adding frequency samples according to Algorithm ISR. The number of samples needed to obtain satisfactory accuracy has to be scaled by the computational cost to evaluate  $f(z)$ . The single-threaded time spent to evaluate the scattering problem at one complex frequency is displayed in Figure 3c for different truncation orders  $m_{\max}$ . The shown error is the maximum relative error amongst thirteen resonances falling in the considered domain of the complex frequency plane between  $(1.6 - 0.4i)$  and  $(2.7 + 0.1i)$  eV. The error is dominated by the T-truncation from ca. 70 samples onwards for moderate  $m_{\max}$ .

In Section S3 (Supporting Information), we compare the found resonances to the results of a state-of-the-art eigensolver based on Arnoldi iteration, which is part of the commercially available finite element method (FEM) software package JCMsuite. The resonance frequencies found by the AAA approximation converge to the reference solution with a remaining maximum relative error of  $\sim 10^{-9}$ , which is within the expected accuracy of the FEM solution (see Figure S1b, Supporting Information).

Considering the combination of Figure 3b, and 3c reveals the trade-off between computational effort and accuracy of our method. For example, a desired accuracy of  $1 \times 10^{-9}$  would require  $m_{\max} \geq 7$  with approximately 85 frequency samples, resulting in a total single-threaded execution time of less than 2s. Comparing that to the Arnoldi iteration, which takes more than 200 s for the same accuracy (Figure S1b, Supporting Information), we observe a computational advantage of about two orders of magnitude for the system at hand. For larger systems, especially in 3D, our proposed method should offer even further savings in computational cost. Furthermore, the computational complexity



**Figure 4.** Modes of a large composite resonator made of 30 cylinders. The central figure shows the complex resonance frequencies of the modes, and the plots above and below show the corresponding field distribution of a few selected modes. Only the dominating  $E_x$  component is shown in these field plots. A few magnified fractions of the images illustrate the symmetries in the field plots. The scalarized response function  $f(z)$  is chosen as a linear function of the scattered field (Scheme 2.1 in Figure 2) under dipole excitation with variable position. When the source is placed in the resonator such that it possesses an even symmetry, modes of odd symmetry along the same axis are suppressed (gray lines indicate odd symmetry, green indicates even in the  $x$ -direction, orange indicates even in the  $y$ -direction). In the legend of the central figure, the axis is set in bold when the source is placed in a high symmetry position relative to that axis and a normal font when not.

of the TMF generally reduces for a wider spacing of the scatterers (because a lower  $m_{\max}$  is needed to capture near-field interaction accurately).

### 3.2. Modal Fields

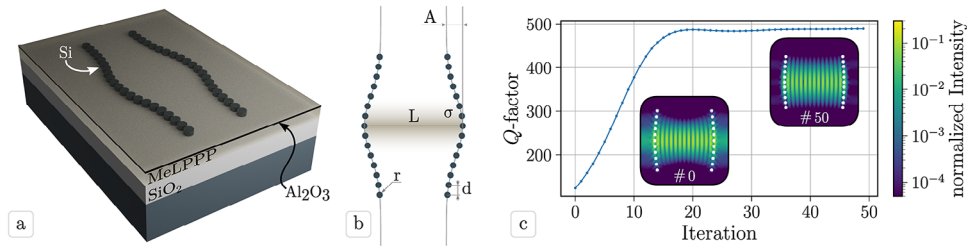
Besides its resonance frequency, a mode is characterized by the corresponding field distribution. As shown in ref. [46], it is possible to construct the modal fields by a weighted superposition of the fields at the sample frequencies  $z_k$ . This is equally possible when the fields are expressed in the VSW/VCW-basis. However, in contrast to ref. [46], we do not necessarily calculate  $f(z)$  as a linear function of the scattered field. Therefore, we evaluate the modal fields using a single scattering simulation close to the pole of interest. The response to any source that couples to a non-degenerate mode will take the form of such mode when the excitation frequency approaches the resonance frequency of the mode.<sup>[59]</sup> We further note that for increased efficiency, only the scattered field distribution has to be evaluated, as it will dominate over the incident field when approaching the pole.

As demonstrated numerically in Section S3 (Supporting Information), the modal fields converge to the state-of-the-art reference eigensolver with the exception of the fields very close to the cylinders. The observed error has more than  $m_{\max}$  oscillations around the scatterers and decreases in magnitude when increasing  $m_{\max}$ . It is thus attributed to the error introduced by the truncation in the multipolar order. The fields shown in Figure 3a and in further figures were calculated with that approach.

### 3.3. Selective Excitation

Let us now move on to a more complex resonator comprising 30 scatterers. The scatterers are placed in 200 nm steps to form two opposing meta-mirrors with a distance of 5200 nm. The material model for silicon is replaced in favor of a nondispersive  $\epsilon_r = 17.77 + 0.2j$ . All other parameters are as given in the first example. The resonator supports a rich spectrum of modes as shown in Figure 4. The central scatter plot contains the positions of the found resonances in the complex frequency plane for different excitations (indicated by different markers). The corresponding electric field distributions are illustrated above and below the scatter plot for two sets of resonances, which are grouped by the number of nodes along the horizontal  $x$  direction (this grouping is also displayed in the scatter plot by the thick strokes). Even symmetries in the modal fields are indicated by a colored symmetry axis (green for  $x$ -, orange for  $y$ -symmetry), while a gray axis indicates odd symmetry. The three magnified regions shown on the right of Figure 4 serve to visualize the described symmetries.

Robustly recovering the rich resonance spectrum involving a large number of modes is enabled by the adaptive refinement strategy described in Algorithm ISR. It can be further helped by deliberately suppressing unwanted modes, which is possible by an appropriate choice of the scalarized response function  $f(z)$ . Here,  $f(z)$  is chosen as one coefficient of the scattered field  $p_{\text{local}}$ , under illumination from an electric dipole inside the cavity. The symmetry of the source inside the resonator is selectively broken by offsetting it from the center.



**Figure 5.** Inverse design of integrated polariton cavity formed by silicon cylinders for maximum  $Q$ -factor. The ladder polymer MeLPPP supports exciton-polaritons when placed in a resonator with sufficient  $Q$ . a) Layer stack for SOI chip integrated polariton cavity. A slab mode guided in the active MeLPPP layer is confined laterally by high contrast gratings formed from silicon posts. A thick layer of buried oxide isolates the resulting resonator from the silicon substrate. b) The posts' positions are parameterized by a Gaussian curve with variable amplitude  $A$ , standard deviation  $\sigma$ . Further free parameters are the center-to-center distance of the posts  $d$  and the mirror distance at the cavity center  $L$ . The posts radius is fixed to  $r = 55\text{nm}$ . c) The evolution of the  $Q$ -factor with optimization iterations. Insets show the modal fields as an intensity distribution with a logarithmic colormap, allowing to clearly identify the radiative loss in the unoptimized geometry. After the optimization concludes barely any radiative loss remains visible.

All modes couple to the source with broken symmetry in  $x$  and  $y$  (i.e., the grey  $\times$  is present for all resonances). Excitations symmetric along one or more axes do not couple to modes antisymmetric along these axes. The orthogonality between excitation and mode becomes apparent by the absence of the respective pole. The divergent entries of the  $\mathbf{T}_{\text{local}}$ -matrix are canceled in  $\mathbf{T}_{\text{local}}\mathbf{a}_{\text{local}}$ , while all entries of  $\mathbf{a}_{\text{local}}$  are non-zero. This can be understood as the extreme case of a vanishing residue due to a mismatch between excitation and mode. During the inverse design presented in the last section, we will analogously use the residue as a similarity measure between source and mode, to pre-select relevant resonances.

### 3.4. Inverse Design

As mentioned in Section 2.2, the AAA algorithm allows us to calculate the gradients of the resonance poles. At the same time, gradients of the Mie coefficients and the TMF can be obtained via automatic differentiation. Thus, it is possible to efficiently differentiate the full solver chain with respect to, e.g., material parameters, geometry, and position of the scatterers. The availability of such gradients unlocks the efficient inverse design of modes of resonators made from multiple scatterers. Let us now demonstrate the inverse design of a photonic microcavity as employed for integrated polariton transistors,<sup>[13]</sup> with meta-mirrors consisting of silicon pillars. The top-down nanofabrication allows the accurate placement of the silicon pillars on demand. Therefore, the inverse design of the pillar arrangement opens the opportunity to suppress surplus optical losses of the photonic cavity resonance (i.e. increase the quality factor  $Q = -\Re\{\tilde{z}\}/2\Im\{\tilde{z}\}$ <sup>[60]</sup>), which is critical to enable exciton-polariton condensation.<sup>[13]</sup>

Making the layered structure shown in Figure 5a accessible to our method requires reducing it to constituents of high symmetry. Here, this is possible using an effective index approximation, which permits the description of the silicon posts as infinitely extended cylinders in a homogeneous background. As shown in Section S6, the found modes and their relative positions agree with the experimental results for the right choice of effective dispersive permittivities. However, the effective index approximation has the limitation that out-of-plane radiation losses are not considered. Such a limitation could be circum-

vented phenomenologically, e.g., by adding a shell of a lossy material around each post. To ease reproducibility, we, however, keep the same permittivities as in the previous example, which approximately coincide with the calibrated effective refractive indices at  $z = 2.5\text{eV}$ .

To keep the complexity of this demonstration to a minimum, we will fix the posts' radius to  $R = 55\text{nm}$ , while the positions are parameterized to follow a Gaussian mirror shape inspired by ref. [13] (see parameters indicated in Figure 5b). Indeed, the Gaussian parameterization is sufficient to reach  $Q$ -factors limited by non-radiative losses. The chosen objective function balances two sub-objectives by the weighting factor  $\eta = 1 \times 10^{-2}$ :

$$F_{\text{obj}} = \underbrace{\Im\{\tilde{z}_*\}^2}_{\text{primary}} - \eta \underbrace{(\Re\{\tilde{z}_*\} - \omega_{\text{target}})^4}_{\text{penalty}}. \quad (5)$$

The primary objective is to maximize the quality factor (or, equivalently, to minimize the distance between the pole and the real axis). A penalty term is added to keep the (real) resonance frequency approximately fixed, which ensures the resonance stays inside the search domain. As  $F_{\text{obj}}$  solely depends on the position of the selected pole  $\tilde{z}_*$ , the sensitivities of all other poles do not contribute to the update step.

The resonator geometry changes with every iteration, consequently modifying the resonance spectrum. The gradients generally differ between resonances. Thus, keeping track of the relevant resonance during the optimization is vital. A combination of three strategies accomplishes this.

1. As discussed in Section 3.3, selected resonances are emphasized by an appropriate choice of  $f(z)$ .
2. The resulting residues are combined with  $\Im\{\tilde{\omega}_i\}$  to assign a relevance score to the poles in the considered spectral window (e.g.,  $\text{Rel}(\tilde{z}_*) := \text{Res}(\tilde{z}_*)/\Im\{\tilde{z}_*\}^2$ ).
3. Lastly, to clearly identify the resonance of interest amongst the remaining most relevant resonances, we compare the modal profiles to a reference mode determined for the initial configuration of posts. For numerical efficiency, the comparison is performed by a small set of point evaluations.

The optimization is performed using the Adam stochastic gradient descent algorithm<sup>[61]</sup> with low momentum terms  $\beta_1 = 0.8$

and  $\beta_2 = 0.9$ . Figure 5c shows the evolution of the quality factor  $Q$  throughout the iterative optimization. The optimizer swiftly finds an optimized arrangement of posts, suppressing the in-plane radiation loss through the mirrors. Note how  $Q$  does not increase monotonically due to the momentum terms of the Adam optimizer and the penalty term used to keep the resonance frequency's real part approximately fixed. The insets show how the radiative loss is clearly visible for the initial configuration, with little radiative loss after the optimizer has converged. Section S7 (Supporting Information) discusses the evolution of design parameters throughout the optimization. The optimizer pushes the Gaussian tails outwards, approaching a parabolic mirror shape. To further maximize  $Q$  while reducing the resonator footprint, more degrees of freedom could be unlocked. Possible design freedoms include the individual placement of scatterers and their geometry. Core-shell cylinders or even freeform structures could replace the posts. Here, we refrain from such measures to guarantee compatibility with established fabrication techniques.

From additional simulations selectively suppressing loss channels, we conclude that the loss remaining for the final design is dominated by dissipation, predominantly in the silicon pillars. It should be noted that due to the effective index approximation out-of-plane radiation losses are not considered. To remedy this in the future, we suggest generalizing the proposed method to arbitrarily shaped objects (i.e., cylinders of finite length) and their inclusion in stratified media, which are both compatible with the TMF.<sup>[62]</sup> Careful treatment of the branch cuts emerging from a nonuniform background will be required.

## 4. Conclusion

This contribution introduces an efficient method to calculate resonance frequencies and associated field profiles of composite resonators. The introduced method is most suitable for geometries that are well described by the underlying transition matrix formalism (TMF). It has been demonstrated elsewhere<sup>[63]</sup> that the TMF is capable to faithfully handle finite clusters of thousands of particles. We are confident that these capabilities extend to our method for resonance calculation by AAA approximation. We demonstrated that our method shows good agreement to established eigen-solvers in the presence of dispersive media. The method requires that the electromagnetic material properties can be evaluated at complex frequencies. Fitting tabulated data to material models presents a physically meaningful way to obtain such permittivity models valid on the complex plane. Appropriate fitting algorithms are openly accessible,<sup>[64,65]</sup> and pre-fitted models are available for a wide variety of materials such as  $\text{TiO}_2$  and  $\text{SiO}_2$ ,<sup>[66]</sup> which are commonly used in dielectric nanoparticles, or gold and silver,<sup>[65]</sup> which can support plasmon polaritons.

We demonstrate the use of automatic differentiation, including custom derivatives for the AAA algorithm, to inversely design a composite resonator with the goal of maximizing its  $Q$ -factor. Further, selective excitation and post-selection of relevant modes are used to track the resonance of interest throughout the optimization. In this work, we have applied our method to high symmetry scatterers (core-shell spheres and infinite cylinders), for which the T-matrix is known semi-analytically. To incorporate arbitrarily shaped scatterers in the optimization, an efficient method to evaluate the T-matrix of such scatterers for a

high number of complex frequency samples is needed. A representation of the T-matrix of an isolated scatterer in terms of a few relevant modes could potentially serve that purpose. Numerous applications beyond finite clusters are based on (locally) periodic arrangements, which can be numerically accommodated for in the TMF by infinite lattice sums.<sup>[62]</sup> Such periodic configurations are known to introduce branch cuts in the optical response function, which requires a generalization of the pole finding method. This would additionally allow the incorporation of stratified embeddings and substrates by expanding the field into a finite set of plane waves. The developments presented in this contribution will serve as a foundation for future efforts addressing these open questions.

## Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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## Conflict of Interest

The authors declare no conflict of interest.

## Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

## Keywords

AAA rational approximation, automatic differentiation, inverse design, quasinormal modes, resonances, resonant states, t-matrix

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