Letter

Extending completeness of the eigenmodes of an open system beyond its boundary, for Green's function and scattering-matrix calculations

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The asymptotic completeness of a set of the eigenmodes of an open system with increasing number of modes enables an accurate calculation of the system response in terms of these modes. Using the exact eigenmodes, such completeness is limited to the interior of the system. Here we show that when the eigenmodes of a target system are obtained by the resonant-state expansion, using the modes of a basis system embedding the target system, the completeness extends beyond the boundary of the target system. We illustrate this by using the Mittag-Leffler series of the Green's function expressed in terms of the eigenmodes, which converges to the correct solution anywhere within the basis system, including the space outside the target system. Importantly, this property allows one to treat perturbations outside the target system and to calculate the scattering cross-section using the boundary conditions for the basis system. Choosing a basis system of spherical geometry, these boundary conditions have simple analytical expressions, allowing for an efficient calculation of the response of the target system, as we demonstrate for a resonator in a form of a finite dielectric cylinder.

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Introduction. The optical response of an object to an excitation is determined by its morphology, material, and the surrounding medium. For spherical resonators the response can be calculated analytically and it is widely known as Mie scattering [1], while for an object much smaller than the wavelength one can use the quasistatic approximation [2], or for a weak scatterer Born's approximation [3]. In more general cases, however, numerical methods are needed to solve Maxwell's equation for the scattered field, such as the finite-difference time-domain approach, or the finite-element method in frequency domain [4]. While directly solving Maxwell's equation with well established methods can be straightforward, it can also be computationally expensive, particularly when a large number of different excitations need to be considered, such as illumination over a wide range of incidence angles and wavelengths, which can be the case when modeling bright or dark field microscopy [5,6].

An alternative approach, which emerged in the last decade, expresses the response of the open system to excitation in terms of its resonances, or complex eigenmodes [7–14]. These eigenmodes, also referred to as resonant states (RSs) [7,8], or quasinormal modes [9,10], are a powerful concept as they describe observables, such as transmittance [7,8], optical cross-section [9,11], or Purcell factor [10,12] in a mathematically rigorous and physically intuitive way. Using completeness properties of sets of eigenmodes [15–19], the observables can be expressed as a Mittag-Leffler (ML) series of the Green's function (GF) [7,11,12] or of the scattering matrix (S matrix) [8,14], or they can also appear as a weighted sum over the eigenmodes [9,10,13].

The question of completeness of eigenmodes, that is, whether they form a suitable basis for expansion of other functions, has been recently reviewed in detail for open systems in Ref. [19]. The region of completeness is assumed to be the minimal convex volume containing the resonator formed by the inhomogeneous region of space, assuming a homogeneous background. This assumption has been verified for analytically solvable systems, such as a slab or a sphere [7,15–17,20]. When the eigenmodes of the system are calculated numerically [13], additional numerical modes can appear in the spectrum, for example due to the use of perfectly matched layers in bounded regularized space, or due to the discretization of the differential operator, and including all such modes in the basis of expansion can result in completeness beyond the resonator [21].

While there have been recent attempts to achieve completeness of the RSs in the region outside the resonator, by applying various methods of their regularization [22–26], the completeness of the true, physical RSs is limited to the interior of the resonator. In this Letter, we show that using the resonant-state expansion (RSE) allows us to extend the completeness of the RSs beyond the volume of the resonator, up to the boundary of the basis system. The RSE rigorously calculates the unknown eigenmodes of a target system by using the complete set of known eigenmodes of a system as a basis for expansion [27]. It is capable of treating large perturbations of a resonator [28,29] and of the surrounding homogeneous medium [30], with the accuracy and number of modes N increasing with the maximum magnitude $k_{\max}$ of the complex wave numbers of basis modes included in the expansion [28,31].

The purpose of this Letter is twofold. Firstly, we show that when the modes of a resonator are generated with the RSE, they form an asymptotically complete set over the basis system volume. Particularly, this means that in case of an embedded target system having a smaller volume, we can obtain an asymptotically complete set of its modes, and the ML series of the GF converges to the correct values in regions beyond the boundaries of the target system. Secondly, using the asymptotic completeness of the RSs inside the basis system, we demonstrate the applicability of the scattering theory [11] to nonspherical resonators and, more generally, to resonators with boundaries different from the boundary of a basis spherical system. Previously, the scattering theory [11], based on the RSE and the link between the dyadic GF and the S matrix, was demonstrated for spherical systems only (and for material perturbations only), where the angular momentum quantum number l, magnetic quantum number m, transverse-electric (TE) and transverse-magnetic (TM) polarizations of light are conserved and can thus be separated. Here, we demonstrate the applicability of the theory to systems with cylindrical symmetry mixing the basis modes of different l and polarizations.

Completeness. First, we show that when the eigenmodes of a system are generated via the RSE, they form an asymptotically complete set over the basis system volume, which embeds the target system and thus includes the gap volume between the basis and the target system boundaries. This principally is enabled by additional modes forming in the spectrum alongside the physical resonances of the system, and these additional modes depend on the basis size chosen. To illustrate this, we take a spherically symmetric dielectric system, which can be treated as an effective one-dimensional (1D) problem, with eigenmodes being functions of the radial coordinate r only. The unperturbed basis system has radius R, and we choose the perturbed target system of radius $R_p = 0.7R$, keeping the same permittivity. We calculate the modes in the complex wave number plane with the RSE, and then construct the GF as an ML series over the perturbed eigenmodes, both inside the perturbed resonator ($r < R_p$) and outside of it ($R_p < r < R$).

For simplicity we focus on the TE modes, for which the GF, having in general a dyadic form in 3D, can be represented in vector spherical harmonics (VSHs) by only one nonzero component and has no contribution from static modes [20]. We consider a nonmagnetic, nondispersive, homogeneous dielectric sphere in vacuum as background, for which the electric field $\mathcal{E}(r)$ satisfies the differential equation [20,31]

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} + k_n^2\varepsilon(r)\right)\mathcal{E}_n(r) = 0, \tag{1}$$

where $\varepsilon(r)$ is the permittivity, k is the complex wave number, and n labels different modes. The basis system has $\varepsilon(r) = \varepsilon_s - \Theta(r-R)(\varepsilon_s - 1)$, and the target system $\varepsilon(r) = \varepsilon_s - \Theta(r-R_p)(\varepsilon_s - 1)$, where Θ is the Heaviside step function, and we set the permittivity of the sphere to $\varepsilon_s = 9$ as in Refs. [11,29].

The modes of the basis (dots) and the target system (squares) are shown in Fig. 1(a), alongside with modes calculated with the RSE (crosses) using two different basis sizes $N = 39$ ($k_{\max}R \approx 20$) and $N = 399$ ($k_{\max}R \approx 210$), for $l = 1$,

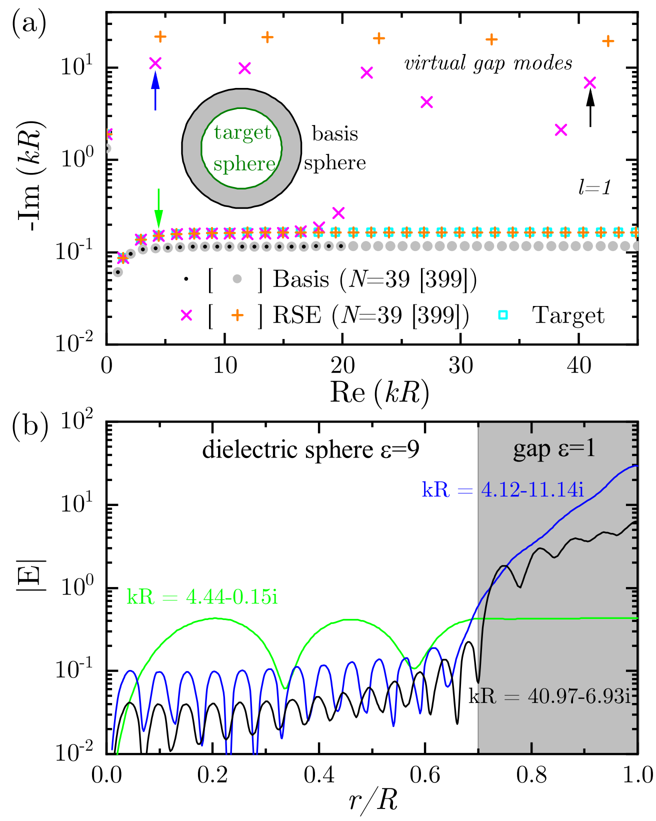

FIG. 1. (a) RSE modes (crosses) of a dielectric sphere with $\varepsilon = 9$, basis radius R, and target radius $0.7R$, in the complex wave number plane, along with the exact modes of the basis (dots) and target system (squares). (b) Field amplitude of a mode close to a physical RS (green) and a lower and a higher order VG mode (blue, black), with arrows in (a) indicating these modes for $N = 39$.

see Refs. [20,27,31] or Sec. S.I of the Supplemental Material [32] for a detailed description of the RSE for this system. We can see that the target modes are correctly calculated via the RSE for wave numbers well below $k_{\max}$, as previously found. Increasing $k_{\max}$ has two effects: increase of the accuracy of modes that were already in the basis range and increase of the range where modes are approximately correctly found [7]. Looking at the results for $N = 39$, we see that apart from modes corresponding to the exact target modes, there are additional modes present in the spectrum, with a significantly larger imaginary part than the exact target modes, even an order of magnitude larger than the single *leaky mode* [31,33] appearing for $l = 1$ on the imaginary axis (for modes with higher l see Sec. S.II of [32]). As such, they have a small amplitude of $\mathcal{E}$ inside the target resonator while growing quickly outside it, as illustrated in Fig. 1(b) and Sec. S.III of [32]. These modes behave as if their fields were weakly reflected from the surface of the basis resonator, which is evidenced by their spectral separation corresponding to the field quantization in the gap region. We will therefore refer to these as *virtual gap modes* (VG modes) in the remainder of this Letter.

For this system the classification of modes as VG modes can be done based on their spectral distance to the exact modes of the target system. While for small $k_{\max}$ the VG modes might be close to leaky modes (see Sec. S.II of [32]), as the basis size tends to infinite, the majority of VG modes tend towards infinite k along the imaginary axis, rather than converge to the true physical modes [see Fig. 1(a)], thus they are clearly distinguishable, except for a few *edge modes* at $Re(k) \approx k_{\max}$. The distance between the real parts of the wave numbers of VG modes is about $\pi/(R-R_p)$, providing over the gap region a phase difference of π between the neighboring VG modes. Consequently, their number for a given $k_{\max}$ grows linearly with the gap size, as detailed in Sec. S.III of [32]. The effect of these modes on the asymptotic completeness of target modes is evaluated by constructing the ML series of the GF of the system.

Following the notation of Ref. [20], the GF $\mathcal{G}$ corresponding to Eq. (1) satisfies the equation

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\varepsilon(r)\right)\mathcal{G}(r,r';k) = k\delta(r-r'), \quad (2)$$

and can be written as an ML series inside the resonator as

$$\mathcal{G}(r,r';k) = \sum_n \frac{k\mathcal{E}_n(r)\mathcal{E}_n(r')}{k_n(k-k_n)}, \quad (3)$$

or

$$\mathcal{G}_{sr}(r,r';k) = \sum_n \frac{\mathcal{E}_n(r)\mathcal{E}_n(r')}{k-k_n}, \quad (4)$$

where the two equations are related by the sum rule

$$\mathcal{S} = \sum_n \frac{\mathcal{E}_n(r)\mathcal{E}_n(r')}{k_n} = 0, \quad (5)$$

as $\mathcal{G}_{sr}(r,r';k) = \mathcal{G}(r,r';k) + \mathcal{S}$.

Now we evaluate the ML series of the GF using modes with wave numbers up to $k_{\max}$ and compare it with the exact GF which can be found from two solutions of the homogeneous wave equation, satisfying the left and right boundary conditions separately [34]; for spherically symmetric systems, a derivation can be found in Ref. [20]. For illustration, we place the source in the gap region at $r' = 0.85R$ and show the results in Fig. 2(a).

First let us consider the ML series over the exact target modes (squares). We can see that well inside the resonator ($r \lesssim 0.6R$) the exact modes are sufficient to reproduce the GF despite one coordinate (r') being located outside the resonator. In fact, when one coordinate is outside, but near the boundary, and one coordinate is inside, away from the boundary, a correct ML expansion using the exact eigenmodes is still possible, due to the analytic GF vanishing for $k \to \infty$ (which is always the case for both coordinates located inside the resonator [15,16]), consistent with findings in Ref. [24], where the same was observed for a slab. If both coordinates are outside, the analytic GF is no longer vanishing for $k \to \infty$, and thus it cannot be written as a correct ML series using the exact eigenmodes only.

Using the modes generated via the RSE including the VG modes in the ML series (crosses), we find that the GF is reproduced correctly across the whole basis system volume, up to R, thus we can conclude that the VG modes dominantly contribute to the completeness in the gap, as confirmed by a detailed analysis in Sec. S.VII of [32]. This is understandable considering that the perturbed modes $\mathcal{E}(r)$ are obtained via a rotation of the basis modes $\mathcal{E}_n(r)$, expressed by the expansion $\mathcal{E}(r) = \sum_n c_n\mathcal{E}_n(r)$, where the expansion coefficients c_n are given by a rotation matrix determined by the RSE matrix equation (see Sec. S.I of [32]), and such a rotation preserves the completeness within the volume of the basis system. Thus, generating eigenmodes via the RSE gives access to the GF also in the gap region (see Sec. S.IV.2 of [32] for a rigorous proof). While one can consider the VG modes as analogues to modes formed by perfectly-matched layers (PMLs) used to describe opens systems [21,35], in the sense that they have an incoming wave component and they provide completeness over a region outside of the resonator [19], they arise for fundamentally different reasons: VG modes form due to the use of basis modes of a larger resonator in an unbounded domain up to a finite maximum frequency, while PML modes form due to the use of an artificially bounded physical domain. We emphasize, that both VG and PML modes are different from numerical modes [21] that arise due to the discretization of the physical space by a mesh in FDTD or FEM solvers.

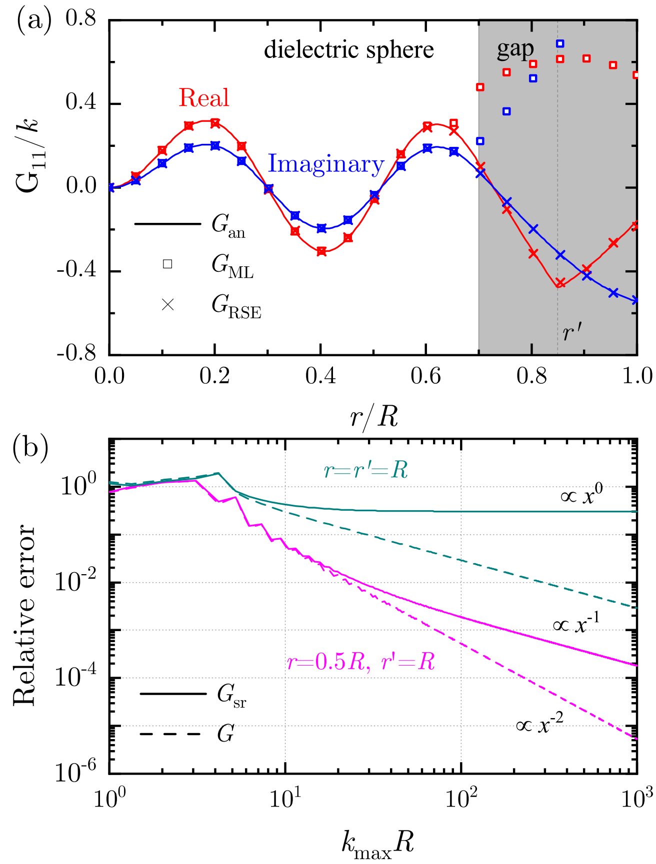

FIG. 2. (a) Comparison of the exact analytic form of the GF ($\mathcal{G}_{\mathrm{an}}$) and its ML series using exact modes ($\mathcal{G}_{\mathrm{ML}}$) with $N = 39$ ($k_{\max}R \approx 28.5$), and modes calculated via the RSE ($\mathcal{G}_{\mathrm{RSE}}$) with $N = 39$ ($k_{\max}R \approx 20$), for a source located in the gap at $r' = 0.85R$ (vertical dashed line), for $kR = 5$. (b) Relative error of the ML series of the GF, with one point and both points on the surface of the basis sphere, as labeled, for $kR = 5$, calculated via Eq. (4) (solid) and Eq. (3) (dashed).

We note that due to the $1/k_n$ factor in $\mathcal{G}(r, r'; k)$, it has a quicker convergence than $\mathcal{G}_{sr}(r, r'; k)$, as illustrated in Fig. 2(b). Such a difference comes from the sum rule Eq. (5) connecting both, which is exact only in the limit of an infinite, complete basis. Notably, $\mathcal{G}_{sr}(r, r'; k)$ does not even converge to the correct solution in the special case of both coordinates at the surface of the basis system, as illustrated in Fig. 2(b), so the summation in $\mathcal{S}$ no longer tends to zero when $r = r' = R$, which is further discussed in Sec. S.IV.3 of [32].

Scattering. We further illustrate the completeness by calculating the scattering cross-section of spherical resonators based on the GF evaluated on their surface, or in the gap volume inside the basis system, including its surface. We apply the method developed in Ref. [11], which is reviewed in Sec. S.V of [32] and consists of: (i) decomposing the incoming excitation into VSHs and TE and TM polarizations; (ii) finding a source term representing the excitation on a spherical surface surrounding the resonator; (iii) for the source term, calculating the response of the resonator from the GF evaluated on this spherical surface; and (iv) from this response, determining the S matrix and the scattering cross-sections. A fundamental result of the method is the link between the S matrix and the dyadic GF [11], which is given by

$$S_{lmp}^{l'm'p'} = G_{lmp}^{l'm'p'}(r_s, r_s; k)\sigma_{l',p'}(k) - \delta_{pp'}\delta_{ll'}\delta_{mm'}, \tag{6}$$

where δ is the Kronecker delta, $G_{lmp}^{l'm'p'}(r, r; k)$ are components of the radial part of the dyadic GF of Maxwell's wave equation for the electric field in the VSH representation, evaluated at the surface of a sphere of radius r_s, while l, m, and p label, respectively, the VSH channels and polarizations of the outgoing waves, with l', m', p' denoting the incoming waves. We note that for a spherically symmetric system, l, m, and p are not mixed and $G(r, r; k) = \mathcal{G}(r, r; k)/(kr^2)$, see Sec. S.VI of [32] for details. The effective source term $\sigma_{l',p'}(k)$ has a simple analytic form due to the use of VSHs and is evaluated at the wave number k of the incoming field. Using the S matrix, we can find the amplitude of the scattered field for each channel (l, m, p), which then allows us to obtain the scattering cross-section σ_{sca}, as detailed in Sec. S.V of [32]. Importantly, the nonresonant background contribution to the S matrix is fully contained in Eq. (6) via the Kronecker delta term and the static pole of the GF, and is not omitted as in Ref. [9], nor does it require further fitting as in Ref. [8], nor approximations as in Ref. [36]. Note that due to the convergence properties discussed above, we need to use the ML series in the form of Eq. (3) for the S matrix in Eq. (6), to ensure its convergence to the correct value, whereas the RSE uses the ML series in the form of Eq. (4) to obtain a linear eigenvalue problem.

We calculate the cross-section of the target system using its own surface, with $r_s = R_p$ in Eq. (6), and using the surface of the basis sphere with $r_s = R$ in Eq. (6). As already mentioned, for a spherically symmetric system, the GF is diagonal, that is, the different channels (l, m, p) do not mix leaving only G_{lmp}^{lmp} nonzero. The cross-section is calculated with and without VG modes and results are shown in Fig. 3(b), with the modes shown in Fig. 3(a).

When the cross-section is calculated on the surface of the target sphere the results with and without VG modes are nearly identical. However, when the cross-section is calculated on the basis surface, which lies outside the perturbed resonator, including the VG modes is essential, as without them the resulting cross-section is an order of magnitude larger and of a different shape. This is consistent with the requirement to include the VG modes in the ML series of the GF for coordinates taken outside the resonator, as seen in Fig. 2. Including the VG modes in the calculation restores the convergence of the ML series, and the results show good agreement with the exact solution. This implies that the scattering formalism developed in Ref. [11] should be suitable in case of nonspherical perturbation as well, where the spherical surface on which G is evaluated can only be chosen outside of the resonator, as we will show below. The effect of excluding selected RSs or VG modes is further discussed in Sec. S.VII of [32], with results showing that RSs far away from the spectral range of interest have a small impact on the accuracy, while all VG modes, particularly in the spectral range of interest, have a significant impact, and cannot be neglected. We note that in this formalism, the static modes, which can be used to represent the static pole of the GF, are crucial for obtaining the correct S matrix and cross-section for nondispersive dielectric systems as opposed to other methods [37,38]. This is due to the quantities being calculated directly from the GF, which has contributions from static modes, adding nonresonant parts to

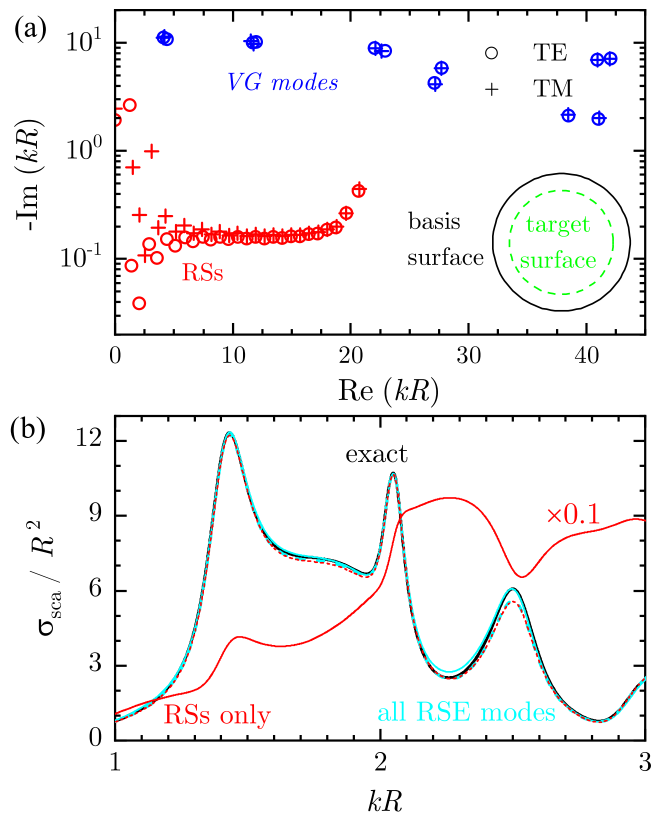

FIG. 3. (a) Complex k-plane with modes of a target dielectric sphere ($\varepsilon = 9$) calculated with the RSE for $l = 1$ and 2, both in TE and TM polarizations, with a basis $k_{\max}R \approx 20$ ($N = 158$). (b) Scattering cross-section of a perturbed sphere of radius $R_p = 0.7R$, with basis modes from a), calculated on the target (dashed lines) and basis surface (solid lines), with (teal) and without (red) VG modes, and the black line showing the exact solution.

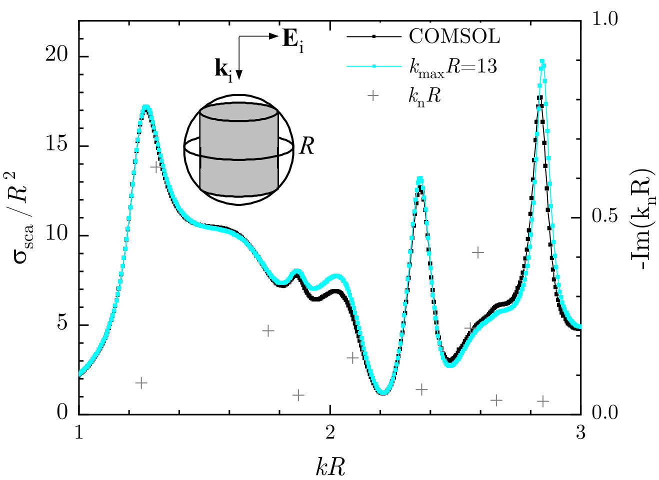

FIG. 4. Scattering cross-section of a cylinder, with $\varepsilon = 9$, height and diameter of $\sqrt{2}R$, and incoming excitation propagating along the cylinder axis ($\mathbf{k}_i$), calculated with $k_{max}R = 13$ ($N = 1004$) and for all l within this frequency range. The eigenmodes in the complex plane are shown for comparison (crosses, right axis).

the S matrix and cross-sections. Leaving out the static mode contribution leads to a considerable systematic error, as shown in Sec. S.VII of [32]. On the other hand, using the RSE allows us to calculate both the RSs and static modes together in the same matrix equation, and therefore does not require a separate static mode solver as in Ref. [38].

Nonspherical systems. We now demonstrate the applicability of the scattering theory also for systems with broken spherical symmetry. We consider a cylinder of equal diameter and height, $\sqrt{2}R$, with $\varepsilon = 9$, as in Refs. [12,29]. The modes of the cylinder are calculated with the RSE (see Sec. S.I of [32] for details) using the RSs of a sphere of radius R as basis. The results are shown in Fig. 4 and compared to a simulation with COMSOL Multiphysics® [39]. We can see good agreement between the two results, which further confirms completeness of the target modes on the original surface of the basis sphere, outside of the cylindrical resonator. A convergence study of the RSE results can be found in Sec. S.VIII of [32], showing that the accuracy improves as more modes are included in the basis, and that the method is computationally efficient.

Conclusion. We have shown that the eigenmodes of a target system generated by the RSE form an asymptotically complete set for ML expansion of the GF over the basis system embedding the target system, including a gap volume surrounding the target. Completeness in the gap volume is due to the presence of VG modes in the spectrum alongside the RSs and static modes of the target system. This allows one to calculate the response to a source in the gap volume, outside the target resonator. As a result, we have found that the scattering theory which links the GF to the S matrix [11] is accurate for a spherical target system, smaller than the basis system with the scattering interface taken at the surface of either the basis or the target system. Importantly, we have extended the application of this scattering theory to nonspherical systems, namely to a cylinder, indicating its validity for arbitrary target systems.

The provision of a complete set of eigenmodes for ML expansion of the GF of an open system in a volume including an adjustable gap region surrounding the system enables important applications in the simulation of open resonators for sources, sensors, and detectors of radiation.

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Data availability. All data supporting this study is openly available in Figshare data repository at [40].

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[32] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevResearch.7.L012035 for details of the method, derivations, and additional data supporting the claims of this letter, containing: Secs. S.I. review of resonant-state expansion; S.II. modes for $l = 10$; S.III. details on VG modes; S.IV. Mittag-Leffler expansion of the Green's dyadic; S.V. scattering matrix in terms of the Green's dyadic; S.VI. Green's dyadic of the Maxwell's equation and of the wave equation; S.VII. effect of modes excluded from the spectra; S.VIII convergence study of the error.
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