Numerical computation of resonance poles in scattering theory

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We present a possible way of computing resonance poles and modes in scattering theory. Numerical examples are given for the scattering of electromagnetic waves by finite-size photonic crystals.

Resonance poles are the main quantity of interest in scattering theory [1,2]. They are poles of the scattering matrix, and may be considered as generalized eigenvalues to which generalized eigenmodes are associated. These poles are complex ones, i.e., they correspond to complex values of the energy in the scattering theory of the Schrödinger equation and to complex frequencies for the scattering theory of the Maxwell system. The point of this note is to suggest a possible way for computing the resonance poles and the associated residues. We must note that there is a rich literature concerning the computations of the poles and zeros of analytic functions (see, for instance, the excellent book by Kravanja and Van Barel and references therein [3]). The situation that we deal with is rather different because the point at issue here is to compute the poles of a meromorphic matrix $z \to T(z) \in M_n(\mathbb{C})$ (i.e., the vector space of $n \times n$ matrices with complex entries), whose entries are not known explicitly, consequently the methods developed for functions have to be adapted.

When dealing for instance with finite-size photonic crystals, i.e., periodic arrangements of scatterers that are finite in at least one direction of space [4], one cannot use the Bloch waves theory to compute the electromagnetic properties of the structure and one has to retreat to the computation of the scattering matrix, i.e., the operator $S(k)$ such that $U^d = S(k)U^i$, where U^i is the incoming part of the field and U^d is the outgoing part of the field and k is the wave number. The scattering matrix writes $S(k) = I_d + T(k)$, where $T(k)$ is the so-called scattering amplitude. Let us assume that there exists some pole k_p of T in some neighborhood $\mathcal{V}$ of the complex plane, then locally the scattering amplitude writes $T(k) = P_p/k - k_p + T_0(k)$, where P_p is a residue operator and T_0 is holomorphic in $\mathcal{V}$. The operator P_p is a finite rank operator and its range, i.e., the vector space in which P_p takes its values, is precisely the nullspace of $T^{-1}(k_p)$ [i.e., the vector space over which $T^{-1}(k_p)$ is null]. Mathematically speaking, we have $T^{-1}(k_p)P_p \equiv 0$. The operator P_p is defined in an abstract way as the Cauchy integral:

$$P_p = \frac{1}{2i\pi} \oint T(z)dz, \qquad (1)$$

where integration takes place on a loop oriented in the direct sense enclosing the only pole k_p. Another way of defining the projection operator P_p is to define it as the following limit:

$$P_p = s - \lim_{k \to k_p}(k - k_p)T(k). \qquad (2)$$

The point of this note is to show that the first abstract definition (1) can be turned into a useful numerical tool for both the computation of the value of the pole and of the residue operator, and hence the generalized eigenmode, whereas the second is useless. From a numerical point of view, we of course only deal with finite rank operators and the scattering amplitude admits a representation as an operator on $l^2(\mathbb{Z})$, i.e., as a matrix, in the usual meaning, acting on double complex sequences [5,6]. Once this representation is given, the residue operator can be computed, provided that a region of the complex plane containing only one pole can be isolated. This means that it suffices to know the value of the pole with a very poor precision to be able to compute the residue operator, which is not the case when the second definition (2) is used; in that last case, numerical instabilities necessarily occur as it uses the product of a singular matrix by a term tending to zero, which is a very bad numerical situation. From a practical point of view, one has to define a path $\gamma : t \in [0,1] \to \gamma(t) \in \mathbb{C}$ whose graph is a loop enclosing k_p and to compute numerically the matrix integral $\int_0^1 T[\gamma(t)]\gamma'(t)dt$ for which any reasonable numerical method works. However, a precise computation of the pole is useful when one wishes to compute a map of the electromagnetic field of the pole, for in that case a particular basis such as Hankel-Fourier series are used, i.e., the field is expanded on the basis $[H_n^{(1)}(k_p r)\exp(in\theta)]_{n \in \mathbb{Z}}$ [5,6]. A possible way is to use a Müller-like algorithm [7] and to compute a zero of the determinant of $T^{-1}(k)$. Unfortunately, this matrix is generally badly conditioned and a better idea is to compute the smallest eigenvalue of $T^{-1}(k)$. However, such an algorithm is not designed to localize the pole, i.e., it is necessary to have a good first guess of the pole for the algorithm to work properly. In order to find a first approximation, we suggest computing the following Cauchy integral:

$$\frac{1}{2i\pi} \oint zT(z)dz = k_p P_p. \qquad (3)$$

Recalling that P_p has finite rank and hence has only a finite number of eigenvalues, a simple comparison of this last integral with P_p gives the value of k_p with a very good accuracy, this last value can then be used in a Müller or Newton-like algorithm to refine the value [8]. Of course formula (3) only holds when k_p is a pole with multiplicity 1; this case is a very common one (see Ref. [11] for practical applications).
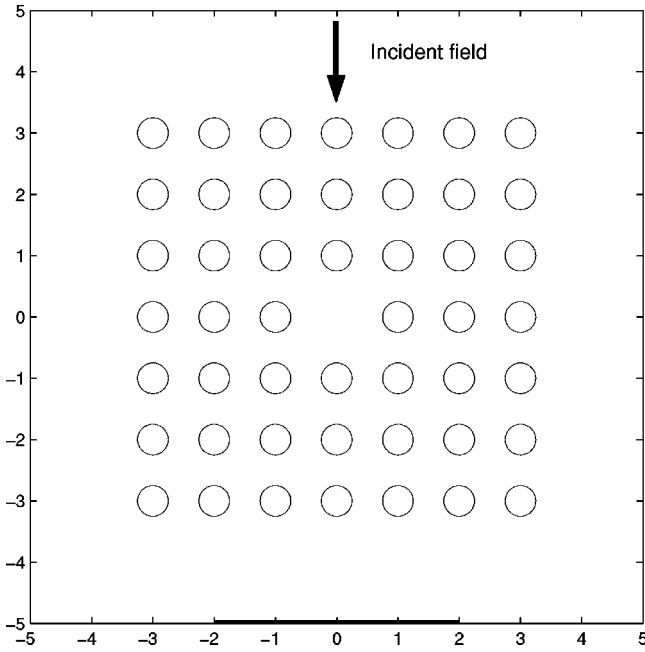
FIG. 1. Sketch of the two-dimensional photonic crystal. The transmission ratio is computed as the flux of the Poynting vector through the segment indicated below the crystal.

One should not mistake the range of P_p with the multiplicity of k_p; it is possible that the multiplicity of k_p is one while the rank of P_p is greater than one [9].

The general case of a pole with multiplicity higher than one occurs when the residue associated with pole k_p cannot be put in diagonal form; this situation can be remedied by adding an infinitesimally small perturbation to P_p, which allows us to split the degenerated levels. The method would work for poles of multiplicity greater than one [3,10] in case of a meromorphic function; it does not work here because we deal with meromorphic matrices.

Let us now turn to some numerical applications. We deal with the structure depicted in Fig. 1. It is a collection of
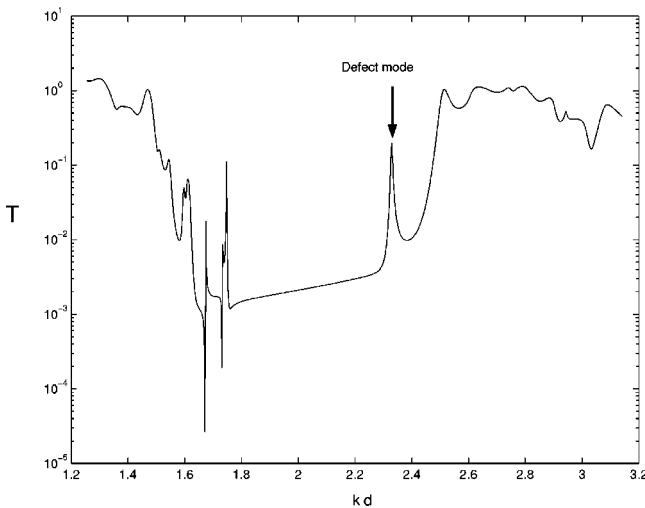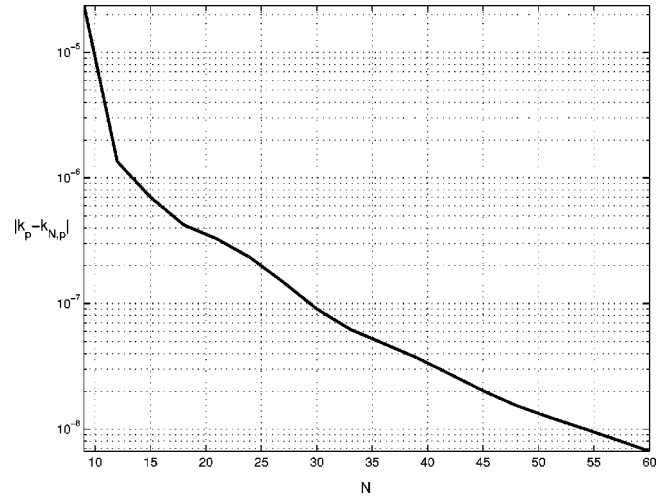

FIG. 3. Convergence of the value of the pole vs the number of integration points.

7×7 homogeneous fibers with relative permittivity $\varepsilon = 9$, the radius of the rods $R = 1/4$, and the spacing is $d = 1$ (these values are given in arbitrary units). We use a rigorous modal theory of diffraction to compute the scattering matrix of this system [5,6]. All the numerical results have been obtained using a standard PC. Removing a rod at the center of the crystal, a defect mode appears in the gap [11] (see Fig. 2 for the transmission spectrum). A pole k_p corresponds to this peak in the transmission spectrum. The reference value that we use for convergence comparison is $k_p = 2.329\,197\,035\,861\,34 - 0.003\,782\,679\,876\,14i$. This value has been computed using the Müller algorithm by minimizing the smallest eigenvalue of T^{-1}. For this given value of k_p, the smallest eigenvalue has modulus inferior to 10^{-14}. We then compute both Cauchy integrals (1,3). The integration path is a triangle whose vertices have affixes (2.3, $2.4 - 0.1i$, 2.4). We use the integration algorithm described in Ref. [12] and we denote by $k_{N,p}$ the numerical value obtained by using N points of integration, which we
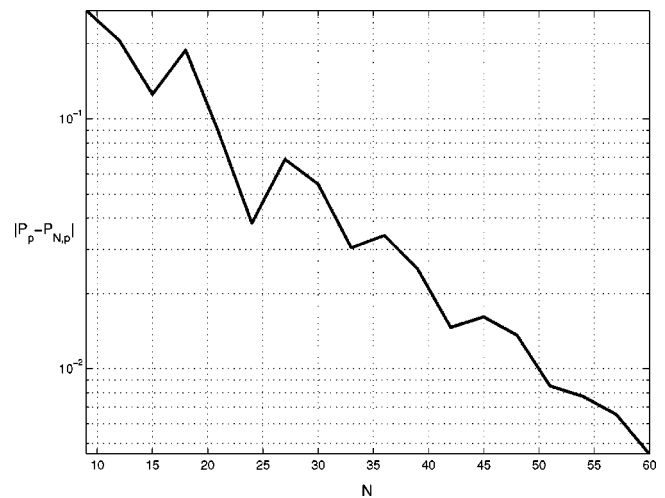

FIG. 2. Transmission ratio vs the dimensionless wave number for an incident plane wave.

FIG. 4. Convergence of the eigenvalue of the projection operator vs the number of integration points.

compare with the above value k_p, which is the best numerical value that we can obtain. A very good precision is rapidly obtained (see Fig. 3); for instance, using a discretization of 15 points, we obtain 6 exact figures, though with such a rough discretization we only get an operator P_p with a low precision. In fact, it seems that the proportional coefficient between both integrals is not very affected by the precision with which P_p is computed. A finer computation of integral (1) gives the defect mode. The convergence can be checked by looking at the nonzero eigenvalue of P_p (Fig. 4), here the reference eigenvalue (i.e., the best numerical value for a pre-

cision error of 10^{-15}) is obtained with $N=150$. A much finer discretization than in the case of the pole is required to get a good representation of the defect mode, though the computing time is perfectly accessible with a very basic PC.

In conclusion, we have shown that it was possible to turn a rather abstract mathematical object into a useful numerical tool. This technique applies as well for any situation in which a meromorphic operator with nonessential poles is involved, which is the usual case. It can serve as an initial step for a Newton or Müller algorithm because it allows a very good localization of a pole.

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