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Determination of quasinormal modes in leaky cavities by diagonalization

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Abstract. Quasinormal modes (QNMs) inside a leaky cavity are characterized by eigenfunctions that are purely outgoing at infinity, and by eigenvalues that are discrete and complex. Apart from a few special cases that admit analytic solutions, the determination of the complex eigenfrequency Ω and the associated eigenfunction $\Phi(x)$ of QNMs is, in general, more difficult than the corresponding case of stationary states, and the various methods have their respective strengths and weaknesses. In this paper, a suitable complete basis set, respecting the outgoing wave condition, is introduced to represent the quasinormal modes in a given system, and a matrix equation is then obtained. It is shown that truncation of this matrix system leads to an efficient and accurate method for solving the eigenvalues and eigenvectors of QNMs.

1. Introduction

Quasinormal modes (QNMs) or resonances are often important in atomic and nuclear physics (Schrödinger's equation) [1], optics (the wave equation with a position-dependent dielectric constant) [2–7], and even gravity [8] (linearized waves on a non-trivial background, described by a Klein–Gordon equation, for example). They may be revealed as peaks in the scattering cross section, or as long-lived states in decay processes [1]. Mathematically, they are time-independent solutions of the respective equations describing open systems and characterized by (i) the outgoing wave boundary condition at infinity, and (ii) a complex frequency Ω with $\mathrm{Im}\,\Omega < 0$. As a consequence, wavefunctions of QNMs blow up exponentially at infinity, and cannot be normalized in the usual sense. Owing to these special features, QNMs are not amenable to the conventional manipulations developed for conservative (Hermitian) systems. For example, completeness, orthogonality and perturbation series are usually established for square-integrable functions; it is not obvious that these relations would hold for QNMs.

Thus, apart from a few special cases that admit analytic solutions, the determination of the complex eigenvalue Ω and the associated eigenfunction $\Phi(x)$ is, in general, more difficult than the corresponding case of stationary states, and various methods all have their respective strengths and weaknesses.

For quantum systems with potentials $V(x)$ that can be analytically continued in x, a rotation in the x-plane can convert the QNM problem into a stationary state problem (but with a complex potential); the usual techniques can then be applied [9]. However, this method is of limited utility for general $V(x)$. In optics, the dielectric constant distribution $\epsilon(x)$ plays a role similar to $V(x)$, and there are often discontinuities representing interfaces, thus preventing analytic continuations.

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QNM problems can also be turned into bound-state problems by enclosing the system in a box of size $\Lambda \gg a =$ characteristic length of the potential, and either by examining the density of states for large Λ [10, 11], or by requiring the stability of the eigenvalues with respect to changes in Λ [12]. This method works well in some cases, but is not likely to be effective for broad or overlapping resonances. Moreover, the QNMs of the original open system are expected to be spaced in wavenumber by $\Delta k \sim \pi/a$, whereas the eigenvalues of the system in the box are $\Delta k \sim \pi/\Lambda$. With $\Lambda \gg a$, the computational effort is increased, and the method could be cumbersome.

Variational methods for QNMs are based on stationarity rather than minimality of an integral, and, moreover, are difficult to improve in a systematic way [9]. Perturbation methods starting from an approximate bound-state problem are necessarily restricted to narrow resonances [13].

An obvious technique is to choose a trial value of Ω, and integrate $\Phi(x)$ numerically to large x. Then Ω is varied until the asymptotic solution satisfies the outgoing wave boundary condition. It is necessary to vary both $\mathrm{Re}\,\Omega$ and $\mathrm{Im}\,\Omega$, but much more seriously, the boundary condition requires that there is no incoming wave. But since $\mathrm{Im}\,\Omega < 0$, the incoming wave is asymptotically the *small* term, whose amplitude is intrinsically difficult to extract from the numerical solution. In contrast, it is relatively easy to extract the amplitude of the *large*, exponentially growing term from a numerical solution, and set it to zero in order to find a stationary state. This difficulty becomes especially serious for broad resonances, because the ratio of the large and small solutions is exponential in $|\mathrm{Im}\,\Omega|$.

A powerful method, useful in many situations, is to expand the required solution $\Phi(x)$ in some basis $\{\phi_j(x)\}$:

$$\Phi(x) = \sum_j a_j \phi_j(x) \tag{1.1}$$

and to convert the eigenvalue problem into a matrix equation for the coefficients a_j. Upon truncation, the problem is then readily solved by standard mathematical packages. This method is not intrinsically restricted to narrow resonances, and, moreover, can give many QNMs simultaneously (in principle, up to N QNMs for an $N \times N$ truncation of the matrix).

The central issue is the choice of a natural and optimal basis set $\{\phi_j(x)\}$ for this purpose. The problem is that, traditionally, the only known complete sets are associated with *Hermitian* systems, while QNMs are intrinsically *non-Hermitian*. For example, in a half-line problem where $x \in [0, \infty)$, one can divide the domain into an interior part $0 \leqslant x < c$ and an exterior part $c < x < \infty$. In the latter, one assumes that the potential (or the dielectric constant distribution) is sufficiently simple (e.g. a constant) that there is an explicit solution which provides a logarithmic derivative for connecting to the interior solution. In the interior, consider, for example, a basis set $\{\phi_j(x)\}$ defined by a differential operator and satisfying the boundary conditions $\phi_j(0) = 0$, $\phi_j(c) = 0$; these conditions define a Hermitian system and ensure that $\{\phi_j(x)\}$ is complete for the space of all functions $f(x)$ satisfying the same boundary conditions, i.e. $f(0) = 0$, $f(c) = 0$. But the point is that the QNM eigenfunction $\Phi(x)$ does *not* satisfy these conditions; indeed, by its very nature, a QNM does not satisfy the boundary conditions for *any* Hermitian system. Thus the set $\{\phi_j(x)\}$ must be augmented by at least one other basis function in order to represent $\Phi(x)$ in the manner of (1.1), for example, the extra function is needed to ensure $\Phi(c) \neq 0$. The resultant formalism is then slightly messy and unnatural. When the basis set is unnatural, one also expects that the result obtained by an $N \times N$ truncation will not converge rapidly as $N \to \infty$.

The awkwardness in the formalism stems from the mismatch between the non-Hermitian

(i.e. non-conservative) nature of QNMs and a Hermitian basis set. However, it has recently been shown that the QNMs $\{\phi_j(x)\}$ of many open systems S_o are complete for describing outgoing waves [14]; they would then provide convenient and natural basis sets for expanding the eigenfunction $\Phi(x)$ of another open system S. The purpose of this paper is to develop this formalism, and to demonstrate that it works extremely well. The method is effective because it is natural to compare one open system S to another open system S_o; in particular, S_o can often be chosen with physical insight to be close to S, in which case one may expect rapid convergence as $N \to \infty$.

We shall present the formalism in terms of the one-dimensional scalar wave equation, which also describes propagation of electromagnetic waves with zero orbital angular momentum in spherical systems [14, 15]. Generalization to electromagnetic waves with non-vanishing angular momenta in three-dimensional space will be reported elsewhere [16].

We are particularly interested in QNMs of optical systems for the following reasons. QNMs of some mesoscopic dielectric structures, e.g. microspheres, may possess very long lifetimes, and provide strong optical feedback to various nonlinear optical processes [4–6]. It is then possible to construct very tiny optical resonators with extremely high Q-factors based on these mesoscopic dielectric systems, and, in turn, achieve the purpose of miniaturization of optical components. In fact, suggestions have been made to build microlasers on tiny dielectric spheres with radial modulation in refractive indices [17]. However, lifetimes of QNMs are extremely sensitive to fine structures of a system, and may deteriorate significantly upon minor changes in refractive index. For example, the lifetimes of QNMs in a dielectric sphere (a droplet) were found to decrease substantially by the presence of impurities (nanometre-sized latex spheres or bubbles) [18, 19]. The lifetimes of QNMs in a fused silica microsphere were observed to be shortened owing to microdusts and layers of contaminants on its surface [20]. In order to provide guidelines to the fabrication of such optical microcavities, one has to understand how QNMs are affected by the details of the dielectric constant distribution; thus, systematic and efficient methods that determine eigenfrequencies and eigenfunctions of QNMs in various configurations are called for. The diagonalization method outlined in the present paper is one of the attempts in this direction.

The rest of this paper is organized as follows. Section 2 is a brief review of the completeness and orthogonality of QNMs, and we shall make use of these properties to formulate the diagonalization method in section 3. Numerical examples and a comparison with results obtained from second-order perturbation [14] will be presented in section 4. A brief discussion in section 5 will then conclude our paper.

2. Completeness and orthogonality

We shall be concerned with a system S defined by a one-dimensional wave equation,

$$\left[\epsilon(x)\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right]\Phi(x,t) = 0 \tag{2.1}$$

where $\epsilon(x) \equiv n^2(x)$, and $n(x)$ is the refractive index distribution. It is often convenient to think of Φ as the transverse vibrations of a string with linear mass density $\rho(x) = \epsilon(x)$ and placed under unit tension. Such open string systems are well studied [10, 21], and their analogy to optics is well known [7, 22]. We shall deal with a half-line problem ($x \geqslant 0$), with boundary condition $\Phi(x = 0, t) = 0$; this could describe the totally reflecting mirror at one end of an optical cavity, or the origin in cases where x represents the radial variable.

Some realistic optical systems described by (2.1) include the following. The distribution $\epsilon(x) = 1 + M\delta(x - a)$ describes a one-dimensional optical cavity enclosed by a thin slab of high dielectric constant at $x = a$, forming a partially transmitting mirror; this is the classic model of a laser cavity [7, 14, 22]. The QNMs in this case are the 'modes' of the laser. The step function distribution $\epsilon(x) = 1 + (n_1^2 - 1)\theta(a - x)$ describes a dielectric rod, and if the differential operator in (2.1) is modified to include a centrifugal barrier $[-\partial^2/\partial x^2 \rightarrow -\partial^2/\partial x^2 + l(l+1)/x^2]$, then this system is the radial problem for electromagnetic waves (in particular TE modes) in a uniform dielectric sphere of radius a, in the sector with angular momentum l. The latter system exhibits well known resonances in Mie scattering, and has been studied extensively in recent years in the context of laser interaction with microdroplets [2–6].

For a general $\epsilon(x)$, the QNMs are defined by

$$\frac{\partial^2}{\partial x^2}\Phi(x) = -\Omega^2\epsilon(x)\Phi(x) \tag{2.2}$$

with the boundary conditions $\Phi(x = 0) = 0$, and outgoing waves as $x \rightarrow \infty$. Our purpose is to develop a method of solving (2.2) by casting it into a matrix equation in a suitable basis. Here we shall restrict our attention to systems S in which $\epsilon(x)$ approaches a constant as $x \rightarrow \infty$ faster than any exponential. (In practice, we shall only deal with systems for which $\epsilon(x) = 1$ for $x > c$.)

For this purpose, we consider a comparison open system S_o, with a distribution $\epsilon_o(x)$. Its QNMs are defined by

$$\frac{\partial^2}{\partial x^2}\phi_j(x) = -\omega_j^2\epsilon_o(x)\phi_j(x) \tag{2.3}$$

with the same boundary conditions. The comparison system S_o is assumed to be exactly solved, i.e. ω_j and $\phi_j(x)$ are known. (We use lower case letters ω_j, ϕ_j for the comparison system S_o, and upper case letters Ω, Φ for the original system S.)

Furthermore, the comparison system S_o has to satisfy two conditions. (i) $\epsilon_o(x)$ contains a step discontinuity at $x = c$, and (ii) $\epsilon_o(x) = \epsilon(x)$ for $x > c$. (In other words, $\epsilon_o(x)$ also approaches a constant as $x \rightarrow \infty$ faster than any exponential.) Under these conditions, it has been shown [14] that $\{\phi_j(x)\}$ forms a complete set inside $[0, c)$ for functions $f(x)$ satisfying $f(0) = 0$ and the outgoing wave condition at $x = c$. This completeness theorem permits a natural expansion in the manner of (1.1), and provides the starting point for the matrix formalism.

In addition to completeness, we also need an orthogonality relation. It has been shown [14], by the usual manipulations, that the QNMs of (2.3) satisfy

$$\begin{aligned}\langle\langle\phi_i|\phi_j\rangle\rangle &\equiv \int_C \mathrm{d}x\, \phi_i(x)\epsilon_o(x)\phi_j(x) \\ &= \delta_{ij}\end{aligned} \tag{2.4}$$

where the contour C is shown in figure 1; it goes along the real axis from 0 to b, where $b > c$, and then to $-\infty$ in the complex plane as shown. Since $\epsilon_o(x) = 1$ for $x > c$, the solution on (c, ∞) is analytic in x, and can be readily continued to complex x; the wavefunctions vanish at the upper limit along C ($x \rightarrow -\infty$), and this allows the usual manipulations to be carried out. Note that the eigenfunctions $\phi_j(x)$ are complex, and the inner product in (2.4) is defined *without* complex conjugation. The diagonal entries in (2.4) define the normalization and phase convention.

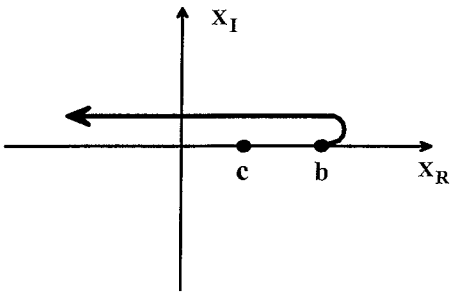

Figure 1. Contour C in the complex x plane for defining the inner product of QNMs. It goes along the real axis from 0 to b, where $b > c$, and then to $-\infty$ in the complex plane x as shown.

With these tools, we are now in a position to cast the original system S into a matrix problem using the basis functions of S_o. A non-trivial feature is that the expansion (1.1) holds only for $0 \leqslant x < c$, but the inner product is defined by the integral (2.4) along C.

3. Formalism

In the rest of this paper, we assume that both the actual system S and the comparison system S_o are trivial outside $x = c$, i.e.

$$\epsilon(x) = \epsilon_o(x) = 1 \qquad x > c\,. \tag{3.1}$$

This condition is sufficiently general (since c can be arbitrarily large) to cover most situations of interest. In particular, in nearly all optical applications, the exterior is vacuum. (The generalization to include the centrifugal barrier $l(l+1)/x^2$ for $x > c$ is somewhat tricky, and will be reported elsewhere.) The difference between the two systems is due to

$$v(x) = \epsilon(x) - \epsilon_o(x) \tag{3.2}$$

which has support on $[0, c)$. Start with (2.2), multiply by $\phi_i(x)$, and integrate from 0 to $-\infty$. (All such integrals will be along the contour C; this will be understood everywhere below.) One obtains

$$\int_0^{-\infty} \mathrm{d}x\, \phi_i(x) \frac{\partial^2}{\partial x^2} \Phi(x) = -\Omega^2 \int_0^{-\infty} \mathrm{d}x\, \phi_i(x) \epsilon(x) \Phi(x)\,. \tag{3.3}$$

On the left-hand side, integrate by parts twice. The surface terms vanish. Then use (2.3) for $\partial^2 \phi_i(x)/\partial x^2$, and obtain

$$\omega_i^2 \int_0^{-\infty} \mathrm{d}x\, \phi_i(x) \epsilon_o(x) \Phi(x) = \Omega^2 \int_0^{-\infty} \mathrm{d}x\, \phi_i(x) \epsilon(x) \Phi(x)\,. \tag{3.4}$$

Separate each integral into the part from 0 to c, and the part from c to $-\infty$; moreover, put $\epsilon(x) = \epsilon_o(x) + v(x)$. Then

$$(\omega_i^2 - \Omega^2) \left\{ \int_0^c + \int_c^{-\infty} \right\} \mathrm{d}x\, \phi_i(x) \epsilon_o(x) \Phi(x) = \Omega^2 \int_0^c \mathrm{d}x\, \phi_i(x) v(x) \Phi(x) \tag{3.5}$$

in which we have used the fact that $v(x) = 0$ for x outside $[0, c)$. In integrals involving wavefunction from $x = 0$ to $x = c$, we are entitled to use the expansion (1.1). For example,

$$(\omega_i^2 - \Omega^2) \int_0^c \mathrm{d}x\, \phi_i(x) \epsilon_o(x) \Phi(x) = (\omega_i^2 - \Omega^2) \sum_j \left\{ \int_0^c \mathrm{d}x\, \phi_i(x) \epsilon_o(x) \phi_j(x) \right\} a_j\,. \tag{3.6}$$

This can be simplified by applying the orthogonality relation

$$\int_0^c \mathrm{d}x\, \phi_i(x)\epsilon_o(x)\phi_j(x) = \int_0^{-\infty} \mathrm{d}x\, \phi_i(x)\epsilon_o(x)\phi_j(x) - \int_c^{-\infty} \mathrm{d}x\, \phi_i(x)\epsilon_o(x)\phi_j(x)$$
$$= \delta_{ij} + \frac{\phi_i(c)\phi_j(c)}{\mathrm{i}(\omega_i + \omega_j)} \tag{3.7}$$

where we have made use of the explicit representation $\phi_j(x) = \phi_j(c)\,\mathrm{e}^{\mathrm{i}\omega_j(x-c)}$ outside $[0, c)$, where $\epsilon_o(x) = 1$.

Similarly, it is readily shown that

$$\Omega^2 \int_0^c \mathrm{d}x\, \phi_i(x)v(x)\Phi(x) = \Omega^2 \sum_j \left\{ \int_0^c \mathrm{d}x\, \phi_i(x)v(x)\phi_j(x) \right\} a_j$$
$$= \Omega^2 \sum_j V_{ij}a_j \tag{3.8}$$

where the matrix element V_{ij} is defined in an obvious way.

Finally, for the integral involving $\phi_i(x)$ and $\Phi(x)$ beyond $x = c$, where QNMs behave as outgoing plane waves, it is trivial to show that

$$(\omega_i^2 - \Omega^2) \int_c^{-\infty} \mathrm{d}x\, \phi_i(x)\epsilon_o(x)\Phi(x) = \mathrm{i}(\omega_i - \Omega)\phi_i(c) \sum_j \phi_j(c)a_j\,. \tag{3.9}$$

Thus, equation (3.5) can be written as the matrix system

$$\sum_j \left\{ S_{ij}\Omega^2 + Q_{ij}\Omega + L_{ij} \right\} a_j = 0 \tag{3.10}$$

where

$$S_{ij} = \delta_{ij} + V_{ij} + \frac{\phi_i(c)\phi_j(c)}{\mathrm{i}(\omega_i + \omega_j)} \tag{3.11}$$

$$Q_{ij} = \mathrm{i}\phi_i(c)\phi_j(c) \tag{3.12}$$

$$L_{ij} = -\omega_i^2 \left\{ \delta_{ij} + \frac{\phi_i(c)\phi_j(c)}{\mathrm{i}(\omega_i + \omega_j)} \right\} - \mathrm{i}\omega_i\phi_i(c)\phi_j(c)$$
$$= -\omega_i^2\delta_{ij} + \omega_i\omega_j \frac{\phi_i(c)\phi_j(c)}{\mathrm{i}(\omega_i + \omega_j)}\,. \tag{3.13}$$

Now S_{ij}, Q_{ij} and L_{ij} are completely determined by the basis set $\{\phi_j(x)\}$, their eigenvalues ω_j, and the potential $v(x)$; in other words they are known. Then equation (3.10) defines an eigenvalue problem for Ω and $\{a_j\}$. This eigenvalue system has certain unusual features, as follows.

(i) The matrices S_{ij}, Q_{ij} and L_{ij} are symmetric but not Hermitian. It follows that Ω is not necessarily real.

(ii) The eigenvalue Ω appears quadratically in the linear system (3.10).

(ii) This linear system can be straightforwardly recast into the form

$$\sum_j \left\{ (\omega_i^2 - \Omega^2)\delta_{ij} - \Omega^2 V_{ij} - (\Omega - \omega_i)(\Omega - \omega_j) \frac{\phi_i(c)\phi_j(c)}{\mathrm{i}(\omega_i + \omega_j)} \right\} a_j = 0 \tag{3.14}$$

from which it is obvious that when $v(x) = 0$, the solutions are $\Omega = \omega_i$, $a_j = \delta_{ij}$.

(iv) If the surface terms $\phi_i(c)\phi_j(c)$ were neglected, equation (3.10) reduces to the usual matrix equation for Hermitian (i.e. closed rather than open) systems.

It will be understood that (3.10) is to be truncated into an $N \times N$ set, so that $\boldsymbol{a}$ is an N-vector, and $\mathbf{S}, \mathbf{Q}, \mathbf{L}$ are $N \times N$ matrices. The appearance of Ω^2 makes it difficult to

utilize standard linear algebra packages. However, this problem is readily surmounted by defining [23]

$$b_j = \Omega a_j \tag{3.15}$$

from which one gets the $2N \times 2N$ system

$$\begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{L} & \mathbf{Q} \end{pmatrix} \begin{pmatrix} \boldsymbol{a} \\ \boldsymbol{b} \end{pmatrix} = \Omega \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{S} \end{pmatrix} \begin{pmatrix} \boldsymbol{a} \\ \boldsymbol{b} \end{pmatrix} \tag{3.16}$$

where Ω appears linearly, and standard routines become applicable.

Since $\Omega \sim \mathrm{i}\partial/\partial t$, the doubling of the variables by (3.16) is equivalent to the usual trick of converting a second-order differential equation into a pair of first-order equations involving (Φ, Ψ), where $\Psi = \partial\Phi/\partial t$. In fact, in such open systems governed by the wave equation, it is natural to consider the simultaneous expansion of (Φ, Ψ) rather than just the expansion of Φ. This aspect is very interesting and will be discussed elsewhere [16].

In general, if N QNMs $\phi_j(x)$ are kept in the basis of expansion, there will be $2N$ solutions to the eigenvalue equation (3.14). However, not all of these $2N$ solutions converge to the exact QNMs of the actual systems S as $N \to \infty$. One has to check whether the solutions satisfy the outgoing wave boundary condition at $x = c$, namely,

$$\left[\Phi'(x)/\Phi(x)\right]_{x=c^-} = \left[\Phi'(x)/\Phi(x)\right]_{x=c^+} = \mathrm{i}\Omega\,. \tag{3.17}$$

Solutions violating this condition will be rejected.

In the next section, we shall apply (3.14) to solve for QNMs of two different systems, and study the accuracy and rate of convergence of the diagonalization method.

4. Numerical examples

In the examples shown below, we use the comparison system with

$$\begin{aligned} \epsilon_o(x) &\equiv n_o^2(x) \\ &= 1 + (n_1^2 - 1)\theta(c - x) \end{aligned} \tag{4.1}$$

to define the basis set for expanding the QNM $\Phi(x)$ of an actual system S described by a more complicated $\epsilon(x)$. To be specific, we take $n_1 = 1.5$, $c = 1.0$ in the following discussion unless otherwise stated. The QNM eigenvalues ω_j and eigenfunctions $\phi_j(x)$ of (2.3) are readily written down [14], namely,

$$\omega_j = \frac{1}{2n_1 c}\left[(2j+1)\pi - \mathrm{i}\ln\frac{n_1+1}{n_1-1}\right] \qquad j = 0, \pm 1, \pm 2, \ldots \tag{4.2}$$

and

$$\begin{aligned} \phi_j(x) &= \sqrt{\frac{2}{n_1^2 c}}\sin(n_1\omega_j x) \qquad 0 \leqslant x \leqslant c \\ &= \sqrt{\frac{2}{n_1^2 c}}\sin(n_1\omega_j c)\,\mathrm{e}^{\mathrm{i}\omega_j(x-c)} \qquad c \leqslant x\,. \end{aligned} \tag{4.3}$$

Note that $\mathrm{Im}\,\omega_j$ are constant and $\mathrm{Re}\,\omega_j$ are evenly spaced.

In the first example, we consider a system S with $\epsilon(x) = \epsilon_o(x) + v(x)$, and $v(x)$ is zero except in the range $a < x < c$, where it is equal to a constant non-vanishing value v_o. In other words, the system S is obtained by 'coating' a thin layer of higher dielectric

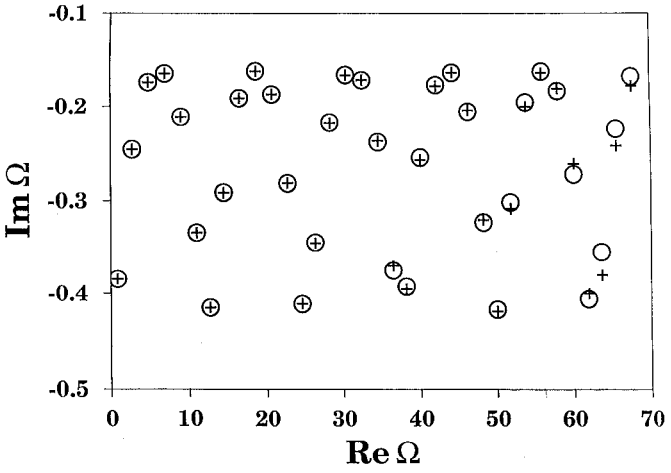

Figure 2. Locations of QNMs in the complex frequency plane for the first example with $v_o = 4.10$, $a = 0.9$, and $N = 100$. Open circles (pluses) show the exact positions (the approximate positions obtained from the diagonalization method) of QNMs. Only modes with $\mathrm{Re}\,\Omega > 0$ are shown; modes with $\mathrm{Re}\,\Omega < 0$ can be readily obtained from the reflection symmetry about the imaginary Ω axis.

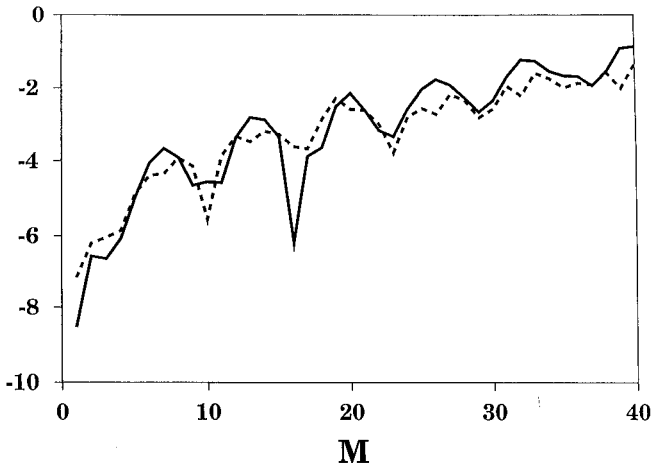

Figure 3. The absolute error (log scale) in the real and imaginary parts of Ω versus the mode number M for the first example with $v_o = 4.10$, $a = 0.9$, and $N = 100$. (i) Logarithm (base 10) of the absolute value of the error in $\mathrm{Re}\,\Omega$ versus M (full curve); and (ii) logarithm (base 10) of the absolute value of the error in $\mathrm{Im}\,\Omega$ versus M (broken curve).

constant on S_o. As $\epsilon(x)$ is piecewise constant, the wave equation is analytically solvable. The resultant eigenvalue equation involves only elementary trigonometric functions and can be solved numerically in a straightforward manner. The exact eigenvalues Ω are denoted by open circles in figure 2, which shows the distribution of the eigenfrequencies on the complex plane. On the other hand, QNM frequencies can also be obtained from the diagonalization method described in this paper by truncating the matrix at a size $N = 100$ [24], and these are denoted by pluses in figure 2. It is observed that the majority of eigenvalues found from the matrix method agrees extremely well with the exact values. The ones near the 'edge' of the

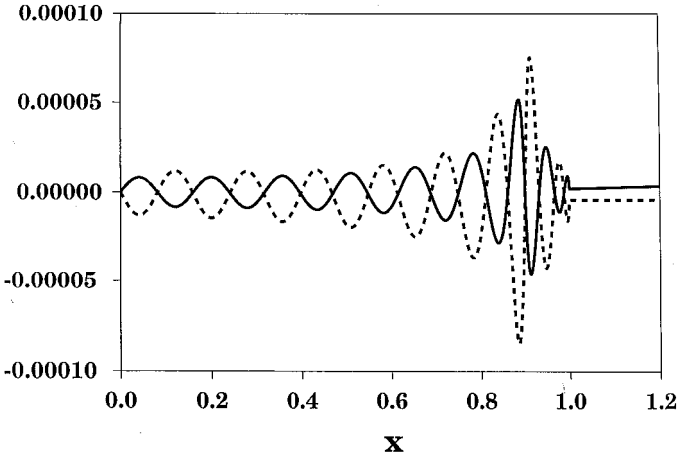

Figure 4. The error in the real and imaginary parts of the wavefunction of the $M = 1$ QNM versus x for the first example with $v_o = 4.10$, $a = 0.9$, and $N = 20$. The full (broken) curve shows the error in the real (imaginary) part of the QNM wavefunction, which is normalized so that $\int_C \mathrm{d}x\, \epsilon(x)\Phi(x)^2 = 1$.

truncation, where $|\mathrm{Re}\,\Omega| \approx$ the maximum of $|\mathrm{Re}\,\omega_i|$ kept in the basis of expansion, cannot be reproduced accurately as expected for obvious reasons; apart from these the results are truly impressive. Note that in this numerical example the perturbation $v_o = 4.10$, and it is even larger than the unperturbed value $n_1^2 = 2.25$. This clearly demonstrates the accuracy and validity of the diagonalization method. Furthermore, the exact eigenvalues Ω of the actual system lie on a sinusoidal locus in the complex plane; this feature is faithfully reproduced by the matrix method. In this case, $|\mathrm{Im}\,\Omega|$ is by no means small (up to 0.4), of the same order of magnitude as the spacing in $\mathrm{Re}\,\Omega$ (approximately 2); thus these resonances overlap considerably. The matrix method works well nevertheless.

Figure 3 shows the error in $\mathrm{Re}\,\Omega$ and $\mathrm{Im}\,\Omega$ versus the order M of the QNM for the truncation size $N = 100$. (The numbering is $M = \pm 1, \pm 2, \ldots$ starting from the smallest $|\mathrm{Re}\,\Omega|$. Only $M > 0$ is shown; the other half is symmetric.) For $|M| < 25$, $\mathrm{Re}\,\Omega$ and $\mathrm{Im}\,\Omega$ are accurate to the level 10^{-2}. The errors in the eigenfrequencies increase gradually with M. As $M \approx 40$, where it is near the 'edge' of truncation, Ω obtained from the diagonalization method are accurate to the level 10^{-1}. Figure 4 shows the error in the normalized wavefunction of the $M = 1$ QNM obtained from the matrix method with $N = 20$—a relatively small basis; both the real and imaginary parts of the wavefunction are accurate to the 10^{-4} level everywhere. Figure 5 shows the error in Ω for the $M = 1$ QNM, versus the size of truncation N, demonstrating very rapid convergence. For this lowest state, a 10×10 truncation gives Ω to the 10^{-5} level. The high accuracy and rapid convergence comes from the fact that the comparison system S_o is close to the actual system S—which is possible only because we use a QNM basis.

In the second example, we take $\epsilon(x) \equiv n(x)^2$, and

$$n(x) = \begin{cases} n_1 & 0 \leqslant x \leqslant a \\ 1 + (n_1 - 1)\cos^2\{[(x-a)/(c-a)]\pi/2\} & a \leqslant x \leqslant c \\ 1 & c \leqslant x\,. \end{cases} \tag{4.4}$$

where $n(x)$ and $n_o(x)$ are, respectively, shown by the full and broken curves in figure 6. This example is interesting since $\epsilon(x)$ and its first-order derivative are continuous everywhere,

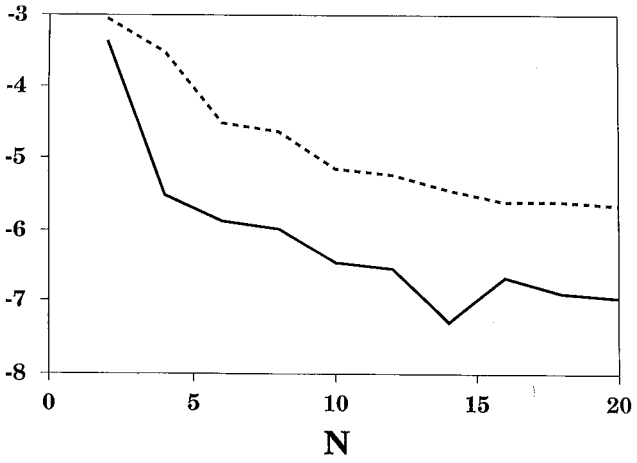

Figure 5. The error (absolute value in log scale) in the frequency of the $M = 1$ QNM, obtained from the diagonalization method for the first example with $v_o = 4.10$ and $a = 0.9$, is plotted against the truncation size N. The full and the broken curves, respectively, show the logarithm (base 10) of the error (absolute value) in $\mathrm{Re}\,\Omega$ and $\mathrm{Im}\,\Omega$.

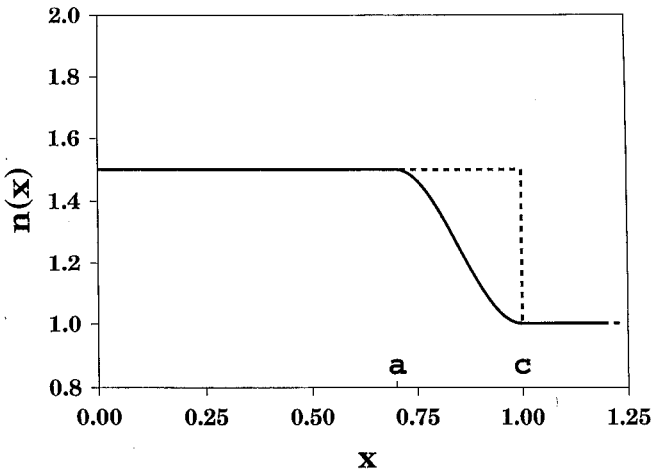

Figure 6. The refractive index distribution for the second example ($a = 0.7$), is plotted against x. The full and the broken curves, respectively, show the refractive indices of the actual system S and the comparison system S_o.

while $\epsilon_o(x)$ of the comparison system has a step discontinuity at $x = c$. As a consequence, the asymptotic behaviour of the QNM frequencies of the two systems are expected to be quite different [14]. This point is clearly demonstrated in figure 7, in which the QNMs of S_o and S (found by numerically integrating the differential equation) are, respectively, denoted by full and open circles. As remarked previously, the imaginary parts of QNMs frequencies of comparison system S_o are constant. By contrast, $|\mathrm{Im}\,\Omega|$ of the actual system S increase as $|\mathrm{Re}\,\Omega|$ increases, and are several times greater than those of S_o. Despite the qualitative differences in the QNMs of these two system, the diagonalization method using S_o as a comparison system nicely reproduces the QNMs of S. The results obtained by truncating

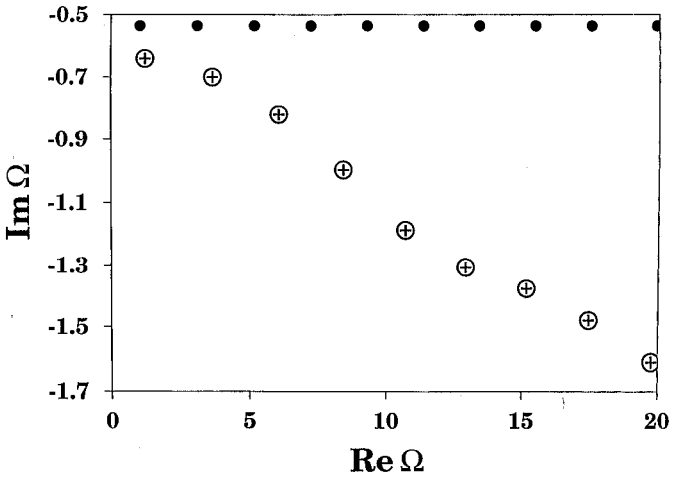

Figure 7. Locations of the QNMs for the second example in the complex Ω plane. The exact positions of QNMs are shown by open circles, while QNMs located by truncating the matrix at a size $N = 20$ are denoted by pluses. In addition, the QNMs of the comparison system are shown by full circles.

at a matrix size $N = 20$ are shown by the pluses in figure 7. The 18 eigenvalues (up to $|\mathrm{Re}\ \Omega| < 20$) shown agree extremely well with the exact values; there is poorer agreement near the edge of the truncation, as expected.

From these two examples one can see that the diagonalization method is very powerful and accurate. Its validity does not depend on whether $\epsilon(x)$ is continuous or discontinuous. In fact, $\epsilon(x)$ can be quite different from $\epsilon_o(x)$, yet results of high accuracy are obtained. Furthermore, the method also applies to systems with rather broad resonances.

One can compare the present method with the perturbative expansion for QNMs developed recently [14]. Consider the first example mentioned above and apply the second-order perturbation theory to evaluate the QNMs by using v_o as the expansion parameter. The error in eigenfrequency of the $M = 1$ QNM is plotted against v_o as shown in figure 8, where results obtained from the diagonalization method and perturbation are denoted by pluses and full circles, respectively. Although the second-order perturbation theory works quite nicely if v_o is small, its accuracy worsens as v_o grows large, as expected. In contrast, the diagonalization method works extremely well for both the small and the large v_o regimes, although the matrix is truncated at a relatively small size, namely $N = 20$. In this respect, the diagonalization method is, in general, much more powerful than the perturbative method.

5. Discussions and conclusion

In this paper we have presented an accurate method—the diagonalization method—to evaluate both the eigenfrequencies and wavefunctions of QNMs. This method has several advantages over the perturbation method developed recently [14]. First, by choosing a proper expansion basis and writing down the corresponding matrix equation, one can readily obtain a set of QNMs of the system under consideration. Second, the accuracy of the diagonalization method is relatively insensitive to the choice of the comparison system, as shown in figure 8. Moreover, one can always improve the accuracy by increasing the size of the matrix as discussed in section 4. In comparison, the validity of perturbation theory

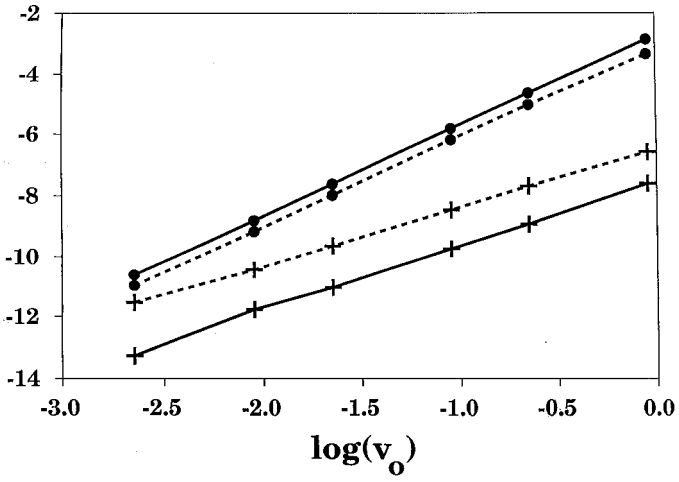

Figure 8. A log–log plot (base 10) of the error (absolute value) in $\mathrm{Re}\,\Omega$ (full curve) and $\mathrm{Im}\,\Omega$ (broken curve) of the $M = 1$ QNM against v_o for the first example with $a = 0.9$ and $N = 20$. Data obtained from the diagonalization method and the second-order perturbation theory are denoted by pluses and full circles, respectively. While numerical computations have been carried out for discrete values of v_o (pluses and full circles), lines (full and broken) are drawn to guide the eye.

relies on the existence of a model system which is on the one hand exactly solvable and, on the other hand, close to the system under consideration. It is often difficult to build an appropriate model system that captures all the details of the original system. Since the asymptotic behaviour of QNMs are, as shown in our previous example, extremely sensitive to the fine structures of $\epsilon(x)$, it is not easy to obtain an accurate perturbative expansion which is applicable over a wide frequency range. In this aspect, the diagonalization method outperforms the second-order perturbation method.

The diagonalization method developed here for QNMs is different from the conventional scheme for bound states in that there is a surface term in the eigenvalue equation. It is this surface term which correctly takes the outgoing wave boundary condition into account. Its emergence in the present paper, in which one-dimensional problems are considered, does not introduce much extra difficulty in solving the eigenvalue equation. However, in dealing with three-dimensional problems, where one has to consider the effect of the centrifugal barrier, the situation is somewhat different. The surface term will involve Hankel functions of the eigenfrequency, which is still to be determined, and renders the numerical solution of the eigenvalue equation non-trivial. Thus, generalization of the diagonalization method to three-dimensional systems is highly non-trivial and will be reported elsewhere.

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References

[1] Goldberger M L and Watson K M 1964 *Collision Theory* (New York: Wiley)
[2] See, e.g., Barber P W and Hill S C 1990 *Light Scattering by Particles: Computational Methods* (Singapore: World Scientific)
[3] Benner R E, Barber P W, Owen J F and Chang R K 1980 *Phys. Rev. Lett.* **44** 475
[4] Snow J B, Qian S X and Chang R K 1985 *Opt. Lett.* **10** 37
[5] Zhang J Z and Chang R K 1989 *J. Opt. Soc. Am.* B **6** 151
[6] Tzeng H M, Wall K F, Long M B and Chang R K 1984 *Opt. Lett.* **9** 499
[7] Lang R, Scully M O and Lamb W E 1973 *Phys. Rev.* A **7** 1788
Lang R and Scully M O 1973 *Opt. Commun.* **9** 331
[8] See, e.g., Chandrasekhar S and Detweiler S 1975 *Proc. R. Soc.* A **344** 441
[9] Ho Y K 1983 *Phys. Rep.* **99** 1 and references therein
[10] Lai H M, Leung P T and Young K 1987 *Phys. Lett.* **119A** 337
[11] Ching S C, Lai H M and Young K 1987 *J. Opt. Soc. Am.* B **9** 1995
[12] Hazi A U and Taylor H S 1970 *Phys. Rev.* A **1** 1109
Mandelshtam V A, Ravuri T R and Taylor H S 1993 *Phys. Rev. Lett.* **70** 1932
[13] Gurvitz S A and Kalbermann G 1987 *Phys. Rev. Lett.* **59** 262
Gurvitz S A 1988 *Phys. Rev.* A **38** 1747
[14] Leung P T, Liu S Y and Young K 1994 *Phys. Rev.* A **49** 3057; 3982
Leung P T, Liu S Y, Tong S S and Young K 1994 *Phys. Rev.* A **49** 3068
[15] See, e.g., Kerker M 1969 *The Scattering of Light* (New York: Academic)
[16] Ng S T 1995 *MPhil Thesis* Chinese University of Hong Kong
[17] Brady D, Papen G and Sipe J E 1993 *J. Opt. Soc. Am.* B **10** 644
[18] Armstrong R L *et al* 1993 *Opt. Lett.* **18** 119
[19] Huston A L, Lin H B, Eversole J D and Campillo A J 1995 Effect of bubble formation on microdroplet cavity quality factors *J. Opt. Soc. Am.* B to appear
[20] Collot L, Lefevre-Seguin V, Brune M, Raimond J M and Haroche S 1993 *Europhys. Lett.* **23** 327
[21] Dekker H 1984 *Phys. Lett.* **104A** 72; 1984 *Phys. Lett.* **105A** 395, 401; 1985 *Phys. Rev.* A **31** 1067
[22] Guedes I and Baseia B 1990 *Phys. Rev.* A **42** 6858
Feng X P and Ujihara K 1990 *Phys. Rev.* A **41** 2668
[23] Press W H, Flannery B P, Teukolsky S A and Vetterling W T 1992 *Numerical Recipes in Fortran* 2nd edn (Cambridge: Cambridge University Press)
[24] Hereafter, by truncating the matrix at a size N, one means that only the N QNMs with the smallest $|\mathrm{Re}\ \omega|$ are kept in the basis of expansion.