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Two-component wave formalism in spherical open systems

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Abstract

We study wave evolution in open dielectric spheres by expanding the wave field and its conjugate momentum—the two components—in terms of relevant quasi-normal modes (QNMs), which are complete under appropriate conditions. We first establish a novel outgoing boundary condition at the surface of a sphere for waves emanating from its interior. A proper definition of inner product for two-component outgoing wavefunctions, involving only the waves inside the sphere and a surface term, can then be defined in general. The orthogonality relation of QNMs and hence a unique expansion in terms of the QNM basis are found, which can be applied to solve for the evolution of waves inside open dielectric cavities. Furthermore, a time-independent perturbation for QNMs can also be developed.

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1. Introduction

Wave evolutions in closed wave systems that are characterized by the nodal (or antinodal) boundary conditions at the walls demarcating a system and its environment are customarily analysed in terms of the associated normal modes (NMs). The eigenvalue problem for NMs in a closed wave system is of the standard Sturm–Liouville type and is governed by a self-adjoint differential operator. Following directly from the self-adjointness of the system, such NMs form a complete orthogonal set and can therefore be used as an appropriate basis to discuss the physics of the system.

However, many wave systems are open, in which energy (or probability) is not conserved, but escape to infinity. Some examples include optical cavities, from which electromagnetic waves can escape (see, e.g. Lang *et al* (1973), Chang and Campillo (1996) and references therein), and regions with curved spacetime around black holes and relativistic stars, from which gravitational waves can escape (see, e.g. Abramovici *et al* (1992)). These physical systems are interesting in their own right and are characterized by the continuous energy-exchange process taking place between them and their environment. In particular, one is often interested in describing how the energy (or probability) inside an open system leaks to its surrounding. However, mathematically speaking, an open system is obviously non-self-adjoint by itself and the usual method of NM expansion is therefore inapplicable. One possible resolution is to embed the system into a 'universe' $0 \leqslant x \leqslant \Lambda$, and impose a nodal condition at $\Lambda \to \infty$, so that the 'universe' as a whole becomes self-adjoint. Then the physics of the system can be discussed in terms of the NMs of the universe. However, one has to work with a continuum of states (spaced by a typical wave number $\Delta k \sim \pi/\Lambda \to 0$) and the concept of the 'modes' of the system, which is intuitively more appealing, is now completely lost. Besides, the non-vanishing coupling between an open system and its environment gives rise to computational difficulty. To simulate the leakage phenomenon, one has to solve the discretized wave equation on a spatial grid extending throughout the system and the environment, which is computationally inefficient. It is more desirable to carry out the simulation with a finite spatial grid covering only the system.

In a series of papers we have proposed a feasible scheme to describe and study the physics of open wave systems solely in terms of relevant quasi-normal modes (QNMs), which are eigensolutions of the wave equation that obey the outgoing-wave boundary condition at the spatial infinity (Leung *et al* 1994a, 1994b, 1997a, 1997b, Ching *et al* 1998). In other words, the wavefunction of a QNM behaves asymptotically as $\exp[\mathrm{i}\omega(x-t)]$ for $|x| \to \infty$, representing monochromatic waves emanating from the system. (Hereafter we will assume that the velocity of wave is unity outside the system for convenience.) The eigenfrequencies ω are complex valued since the system is no longer Hermitian in the usual sense. As energy inside the system is lost continuously to the outside, the amplitude must be decaying in time, leading to the conclusion that $\mathrm{Im}(\omega) < 0$, which in turn shows that QNM wavefunction diverges exponentially at large distances. More importantly, QNM spectra are discrete with a typical spacing $\Delta\omega \sim \pi/a$, where a is the typical size of the system, as in the conservative case. In the limit of zero leakage, the system becomes closed and these QNMs reduce to NMs. These QNMs can be experimentally observed in the frequency domain as resonances of finite widths in the electromagnetic spectrum seen outside an optical cavity (Lang *et al* 1973, Chang and Campillo 1996). Besides, numerical simulations of binary black holes collision show that the gravitational waves generated from such events are dominated, at intermediate times, by damped oscillations, which are precisely the QNMs of the system (Anninos *et al* 1993, 1995).

It is clear that QNMs play an important role in open systems, just as NMs do in closed systems, and it would obviously be useful if the physics of open systems could be discussed, in a precise way, in terms of the discrete QNMs. This method is expected to be computationally efficient and conceptually clear, as opposed to the modes of the universe approach. However, QNMs in open systems in general do not form a complete set for expansion (see, e.g. Ching *et al* (1995, 1996, 1998)). The issue of completeness of QNMs has been the major obstacle hindering the development of QNM expansion. To overcome this difficulty, we and other co-workers have carried out an in-depth investigation along this direction and showed that the QNMs of certain open systems indeed form a complete set (Leung *et al* 1994a, Ching *et al* 1995, 1996, 1998). As an example to illustrate the completeness relation of QNMs, we consider QNMs defined by the wave equation (Leung *et al* 1994a)

$$\left[\epsilon(x)\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right]\phi(x,t) = 0. \tag{1.1}$$

Here $0 \leqslant x < \infty, \epsilon(x) > 0$ plays the role of a position-dependent dielectric constant (or impedance) and $\epsilon(x > a) = 1$ (or other constant). QNMs of this system are defined by the eigen-equation

$$\left[\epsilon(x)\omega^2 + \frac{\partial^2}{\partial x^2}\right]\phi(x,t) = 0, \tag{1.2}$$

where $\phi(x,t)$ has an $e^{-i\omega t}$ time dependence, subject to the boundary conditions (i) $\phi(x = 0,t) = 0$ and (ii) the standard outgoing-wave boundary condition $\phi'(x,t) = i\omega\phi(x,t)$ for $x > a$. (Hereafter we will use a prime to indicate differentiation with respect to the spatial variable x.) This models, for example, an optical cavity with a totally reflecting mirror at one end ($x = 0$) and waves escaping through the other end ($x = a$) to infinity. This system is of course dissipative because of the escape of waves. For such a system we have shown that if there is a discontinuity in $\epsilon(x)$ (or its finite order derivative) at $x = a$, the QNMs form a complete set within the domain $[0, a]$ (Leung *et al* 1994a). For example, the Green's function of the system can be expanded in terms of the associated QNMs inside the finite domain $[0, a]$. In fact, based on the QNM expansion of the Green's function, the time-independent perturbation theory for QNMs has properly been formulated (Leung *et al* 1994b).

However, QNMs are indeed overcomplete and hence an arbitrary function can be expanded in terms of QNMs in infinitely many different ways. This remarkable feature is a direct consequence of the lack of a proper orthogonality relation for QNMs. Consequently, the implementation of standard eigenmode expansion using discrete QNMs cannot proceed in the usual way and is severely limited.

To achieve a unique expansion with QNM basis and seek the physical meaning underlying such expansion, we established a two-component wave formalism for scalar waves propagating in one-dimensional open systems, which are governed by (1.1) (Leung *et al* 1997a, 1997b). In this formalism, the wave equation (1.1) is rewritten in a two-component form

$$\frac{\partial}{\partial t}\begin{pmatrix}\phi(x,t)\\ \hat{\phi}(x,t)\end{pmatrix} = -i\mathcal{H}\begin{pmatrix}\phi(x,t)\\ \hat{\phi}(x,t)\end{pmatrix}, \tag{1.3}$$

where

$$\mathcal{H} = i\begin{pmatrix}0 & 1/\epsilon\\ \partial^2/\partial x^2 & 0\end{pmatrix} \tag{1.4}$$

and $\hat{\phi}(x,t) = \epsilon\partial_t\phi(x,t)$ (Leung *et al* 1997a, 1997b). Correspondingly, the eigen-equation for QNMs is reformulated as

$$\mathcal{H}|\phi\rangle = \omega|\phi\rangle, \tag{1.5}$$

where

$$|\phi\rangle \equiv \begin{pmatrix}\phi(x,t)\\ \hat{\phi}(x,t)\end{pmatrix}. \tag{1.6}$$

It is remarkable that the outgoing boundary condition can now be replaced by $\phi'(x = a^+, t) = -\hat{\phi}(x = a^+, t)$—a frequency-independent equation relating the two components at a finite point $x = a^+$. Therefore, one can see that the introduction of the two-component formalism can indeed simplify the dynamics of such an open cavity as long as there are no incoming waves.

One salient feature of the two-component form of QNMs is that the inner product of the two wavefunctions satisfying the frequency-independent outgoing boundary condition mentioned above can be defined via the bilinear map

$$\langle\varphi|\psi\rangle = \int^{a}[\varphi(x)\hat{\psi}(x) + \hat{\varphi}(x)\psi(x)]\,dx + \varphi(a^+)\psi(a^+). \tag{1.7}$$

Under such definition of the inner product, $\mathcal{H}$ is symmetric (analogue of self-adjoint), i.e. $\langle\varphi|\mathcal{H}\psi\rangle = \langle\mathcal{H}\varphi|\psi\rangle$, which is readily verified. (Hereafter we shall suppress the t-dependence in the wavefunction in cases where there is no ambiguity.) From this property, various results can be obtained in parallel with the familiar formalism for self-adjoint system. In particular, this readily leads to the conventional orthogonal relation of two QNMs, which is defined in the domain $[0, a^+]$. Therefore, any two-component wavefunction $|\psi\rangle$ can be expanded in terms of the corresponding complete set of time-independent QNMs $\{|f_n\rangle\}$, defined by $\mathcal{H}|f_n\rangle = \omega_n|f_n\rangle$, as

$$|\psi\rangle = \sum a_n|f_n\rangle, \tag{1.8}$$

with expansion coefficient given by the usual projection formula

$$a_n = \frac{\langle\psi|f_n\rangle}{\langle f_n|f_n\rangle}. \tag{1.9}$$

More importantly, if a state $|\psi(t)\rangle$ evolves according to (1.3) and $|\psi(t=0)\rangle = \sum a_n|f_n\rangle$, $|\psi(t)\rangle$ can be obtained simply by replacing a_n with $a_n\exp(-\mathrm{i}\omega_n t)$.

In short, the inner product defined in (1.7) allows one to recover nearly all the familiar apparatus of mathematical physics. However, (1.7) is specific to the one-dimensional wave equation (1.1). To see this point, we consider here the radial problem for a three-dimensional spherical system:

$$\left[\epsilon(r)\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{r^2}\right]\phi(r,t) = 0, \tag{1.10}$$

where, as usual, $l = 0, 1, 2, \ldots$ is the angular momentum. In the trivial case $l = 0$, (1.10) is identical to (1.1) and will be ignored in the following discussion. Despite that QNMs of such systems with $l \neq 0$ can be defined analogously and they form a complete set within the region $0 \leqslant r \leqslant a$ under the condition stated above (Lee *et al* 1999), establishment of a two-component formalism for them is tricky. Unlike the one-dimensional case, where the outgoing boundary condition $\phi' = \mathrm{i}\omega\phi$ can be imposed at any $r > a$, such outgoing boundary condition holds only at $r \to \infty$ for non-vanishing l. It is not yet clear how the frequency-dependent outgoing boundary condition at $r \to \infty$ can be replaced with a frequency-independent relation between the two-components at $r = a^+$ (or any finite point $r > a$). Similarly, a proper definition of the inner product is still in question. The main problem is the presence of the centrifugal barrier $l(l+1)/r^2$ that gives rise to finite scattering for $r > a$, where $\epsilon = 1$.

The purpose of this paper is to generalize the two-component formalism to cases with $l \neq 0$, which would then open the way to application to a number of physical phenomena in three-dimensional open systems (Chang and Campillo 1996, Anninos *et al* 1993, 1995). We study specifically the evolution of electromagnetic waves in spherical dielectric open systems, which are described by the vector wave equation

$$\nabla\times(\nabla\times\mathbf{E}) + \epsilon(r)\frac{\partial^2\mathbf{E}}{\partial t^2} = 0, \tag{1.11}$$

where $\mathbf{E}$ is the electric field and for convenience we set $c = 1$ hereafter. This equation follows directly from the source-free Maxwell equations and describes the variation of the electric field $\mathbf{E}$ inside a non-magnetic dielectric sphere characterized by a dielectric constant $\epsilon(r)$. As various interesting optical phenomena have been observed in dielectric microspheres since the eighties (Chang and Campillo 1996) and indeed proposals have recently been made to generate entangled photons in microspheres (Yao *et al* 2004), generalization of the two-component formalism to such systems is deemed necessary and timely. The major achievements of our work reported here are summarized as follows. (i) An outgoing boundary condition relating the two wave components is generally defined at the surface of the system ($r = a^+$). For example, for waves governed by (1.10) the outgoing boundary condition reads

$$[\phi - a\phi' - a\hat{\phi} - a^2\phi'' - a^2\hat{\phi}']_{x=a^+} = 0, \qquad l = 1; \tag{1.12}$$
$$[3a\phi' - 3a^2\phi'' - 3a^2\hat{\phi}' - a^3\phi''' - a^3\hat{\phi}'']_{x=a^+} = 0, \qquad l = 2 \tag{1.13}$$

and a general condition valid for any l can be found in the text. (ii) A proper definition of inner product, involving only the waves inside the system where $0 \leqslant r < a^+$, is defined in general. (iii) The orthogonality relation of QNMs is established. (iv) A unique expansion in terms of QNM basis is obtained, which can be applied to solve for the evolution of waves inside open spherical cavities and time-independent perturbation for QNMs.

The structure of the present paper is as follows. First, the completeness of QNMs in dielectric spheres is introduced as a review in section 2. Second, we formulate the two-component expansion and introduce novel definitions of outgoing waves and the inner product of QNMs in section 3. Third, we establish the associated linear space structure and solve wave evolution in open three-dimensional systems with the two-component formalism in sections 4 and 5 respectively. In section 6 we provide numerical examples to support our theory and in section 7 we show that time-independent perturbation theory for QNMs can be formulated using the two-component formalism. A brief discussion in section 8 concludes the paper.

2. QNMs of electromagnetic waves

To define QNMs satisfying (1.11), we assume a time dependence $e^{-i\omega t}$ of the field, leading to a time-independent vector wave equation

$$\nabla \times (\nabla \times \mathbf{E}) - \epsilon(r)\omega^2\mathbf{E} = 0. \tag{2.1}$$

By virtue of $\nabla \cdot (\epsilon\mathbf{E}) = 0$, the electric field $\mathbf{E}$ can be expanded in terms of the TE and TM modes as follows (Jackson 1975):

$$\mathbf{E}_{1lm} = u_l(r)\mathbf{X}_{lm}(\phi, \theta), \tag{2.2}$$
$$\mathbf{E}_{2lm} = \frac{\mathrm{i}}{\omega\epsilon(r)}\nabla \times [v_l(r)\mathbf{X}_{lm}(\phi, \theta)], \tag{2.3}$$

where u_l and v_l are the radial functions of the TE and TM modes respectively. The angular functions $\mathbf{X}_{lm}$ are the vector spherical harmonics, defined by (Jackson 1975)

$$\mathbf{X}_{lm}(\phi, \theta) = \frac{1}{\sqrt{l(l+1)}}\mathbf{L}Y_{lm}(\phi, \theta), \tag{2.4}$$

where $\mathbf{L} = -\mathrm{i}\mathbf{r} \times \nabla$ and Y_{lm} are the spherical harmonics. It is readily shown that the radial wavefunctions u_l and v_l satisfy the following equation:

$$\left[-\frac{\mathrm{d}}{\mathrm{d}r}\rho(r)\frac{\mathrm{d}}{\mathrm{d}r} + \rho(r)\frac{l(l+1)}{r^2} - \rho(r)\epsilon(r)\omega^2\right]\Psi = 0, \tag{2.5}$$

where $\Psi = ru_l$ ($\Psi = rv_l$) and $\rho(r) = 1$ ($\rho(r) = 1/\epsilon(r)$) for the TE (TM) mode. It is obvious that the TE-mode radial equation is identical to the three-dimensional scalar wave equation mentioned in section 1.

As usual, QNMs of a dielectric sphere are defined as the eigenfunctions of equation (2.5) with the following boundary conditions: (i) the regular boundary at the origin, i.e. $\Psi\ (r = 0) = 0$ and (ii) the outgoing-wave boundary condition at infinity, i.e. $\lim_{r\to\infty}[\Psi(r)\exp(-\mathrm{i}\omega r)] =$ constant. We denote the eigenfrequency and the corresponding eigenfunction of the jth QNM by ω_j and $f_j(r)$, respectively. The QNM frequencies are in general complex with negative imaginary parts and they distribute symmetrically about the $\mathrm{Im}\,\omega$ axis. Such QNMs are also termed as morphology-dependent resonances (MDRs) in the context of light scattering by microparticles (see, e.g. Chang and Campillo (1996) and references therein).

On the other hand, one can also write down a time-dependent wave equation in accord with equation (2.5) as

$$\left[\rho(r)\epsilon(r)\frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial r}\rho(r)\frac{\partial}{\partial r} + \rho(r)\frac{l(l+1)}{r^2}\right]\phi(r,t) = 0. \tag{2.6}$$

As discussed above, this equation governs the propagation of waves (including scalar and EM waves) in spherical cavities and forms the starting point of the ensuing discussion. It also motivates us to consider the retarded Green's function $G(r, r'; t)$, defined by

$$\left[\rho(r)\epsilon(r)\frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial r}\rho(r)\frac{\partial}{\partial r} + \rho(r)\frac{l(l+1)}{r^2}\right]G(r, r'; t) = \delta(r-r')\delta(t) \tag{2.7}$$

and $G(r, r'; t) = 0$ for $t \leqslant 0$. Likewise, the Green's function in the frequency domain, $\tilde{G}$, satisfies

$$\left[-\rho(r)\epsilon(r)\omega^2 - \frac{\partial}{\partial r}\rho(r)\frac{\partial}{\partial r} + \rho(r)\frac{l(l+1)}{r^2}\right]\tilde{G}(r, r'; \omega) = \delta(r-r'). \tag{2.8}$$

Under the conditions that (i) $\epsilon(r)$ has at least a step discontinuity at $r = a$ and (ii) $\epsilon(r) = 1$ (or other constant value) for $r > a$, QNMs are complete inside the region $0 < r < a$ (Leung and Pang 1996, Lee *et al* 1999) and obey the standard completeness relation

$$\frac{\rho(r)\epsilon(r)}{2}\sum_j f_j(r) f_j(r') = \delta(r-r'), \tag{2.9}$$

where the QNMs are normalized in such a way that

$$\lim_{X\to\infty} 2\omega_j \int_0^X \mathrm{d}r\; \rho(r)\epsilon(r) f_j(r)^2 + \mathrm{i} f_j(X)^2 = 2\omega_j. \tag{2.10}$$

Accordingly, the Green's function acquires the following expansion for $r, r' \in [0, a]$ and $t > 0$ (Leung and Pang 1996):

$$G(r, r'; t) = \frac{\mathrm{i}}{2}\sum_j \frac{1}{\omega_j} f_j(r) f_j(r')\,\mathrm{e}^{-\mathrm{i}\omega_j t}. \tag{2.11}$$

It is also worth noting that these QNMs obey an additional sum rule

$$\frac{\mathrm{i}}{2}\sum_j \frac{1}{\omega_j} f_j(r) f_j(r') = 0, \tag{2.12}$$

for $r, r' \in [0, a]$.

3. Two-component formalism

3.1. Two-component waves

As in the one-dimensional case, we define $\hat{\phi}(r, t) \equiv \rho(r)\epsilon(r)\partial_t\phi(r, t)$ and consider the simultaneous expansion of a pair of functions, $\varphi(r) \equiv \phi(r, t = 0)$ and $\hat{\varphi}(r) \equiv \hat{\phi}(r, t = 0)$,

$$\begin{pmatrix}\varphi(r)\\ \hat{\varphi}(r)\end{pmatrix} = \sum_n a_n \begin{pmatrix}1\\ -\mathrm{i}\omega_n\rho(r)\epsilon(r)\end{pmatrix} f_n(r). \tag{3.1}$$

Note that the same set of coefficients a_n are used for both components and the expansion holds inside the system where $r \in [0, a]$. In this paper we shall seek an appropriate definition of the inner product $\langle\varphi|f_n\rangle$ such that the coefficient a_n is still given by (1.9). The physical significance of the two-component expansion is that it can also generate the correct dynamics of the system, namely

$$\begin{pmatrix} \phi(r,t) \\ \partial_t\phi(r,t) \end{pmatrix} = \sum_n a_n \begin{pmatrix} 1 \\ -\mathrm{i}\omega_n \end{pmatrix} f_n(r)\,\mathrm{e}^{-\mathrm{i}\omega_n t}. \tag{3.2}$$

We will justify this claim that holds for 'outgoing waves' in the present paper. However, before establishing the formalism, we have to define what 'outgoing waves' exactly means.

3.2. *Outgoing-wave boundary conditions*

In the case of one-dimensional waves, the space of outgoing waves Γ is defined to be those $(\varphi, \hat{\varphi})$ satisfying (i) the nodal boundary condition at $r = 0$ and (ii) the outgoing-wave boundary condition

$$\hat{\varphi}(r) = -\varphi'(r), \qquad \text{for} \quad r > a. \tag{3.3}$$

This outgoing-wave boundary condition follows directly from the factorization of the one-dimensional wave operator

$$\partial_t^2 - \partial_x^2 \equiv (\partial_t - \partial_x)(\partial_t + \partial_x). \tag{3.4}$$

However, due to the presence of the centrifugal barrier, the wave equation in three dimensions is no longer factorizable and thus the outgoing-wave boundary condition has to be properly modified.

The outgoing-wave boundary condition is very important in the development of the two-component formalism. Physically, it defines the system to be a leaky one. Mathematically, it is used to remove the reference to the outside in the evolution formula, which is the starting point for establishing the QNM expansion. Therefore, in order to generalize the two-component formalism to open spherical cavities, one needs to know how to characterize outgoing waves. We note that spherical outgoing wave solution with a definite frequency ω is given by $g(\omega r)$ for $r > a$, where $g(z) \equiv z h_l^{(1)}(z)$ and $h_l^{(1)}(z)$ is the spherical Hankel function of the first kind. Therefore, in general, the outgoing-wave solution ϕ for $r > a$ can be expressed as

$$\phi(r,t) = \int \mathrm{d}\omega\, \mathcal{A}(\omega) g(\omega r) \exp(-\mathrm{i}\omega t), \tag{3.5}$$

where $\mathcal{A}$ is a function of ω. It turns out that this condition can be used to remove the reference to the outside in the evolution formula.

On the other hand, a deeper physical interpretation to this condition can be unveiled by expressing $\phi(r,t)$ in terms of data of ϕ, $\partial_t\phi$ at an earlier time $t' < t$:

$$\phi(r,t) = \int_0^\infty \mathrm{d}r'\rho(r')\epsilon(r')[\phi(r',t')\partial_{t'}G(r,r';t-t') - G(r,r';t-t')\partial_{t'}\phi(r',t')], \tag{3.6}$$

following from standard application of the Green's function method. If both $\phi(r',t')$, $\partial_{t'}\phi(r',t')$ vanish for $r' > a$, one then has

$$\phi(r,t) = \int_0^a \mathrm{d}r'\rho(r')\epsilon(r')[\phi(r',t')\partial_{t'}G(r,r';t-t') - G(r,r';t-t')\partial_{t'}\phi(r',t')]. \tag{3.7}$$

As the Fourier transform of $G(r,r';t-t')$ is proportional to $g(\omega r)$ for $r > a > r'$, (3.5) can be readily obtained. Therefore, waves obeying the outgoing boundary condition (3.5) are indeed waves emanating solely from the interior of the system, which agrees nicely with our intuitive definition.

The outgoing wave condition (3.5) operates only in the frequency domain. However, based on this we can also derive another equivalent outgoing boundary condition for $r > a$, involving $\phi(r, t)$ and $\hat{\phi}(r, t) \equiv \partial_t \phi(r, t)$, and their spatial derivatives, which will be detailed as follows. To derive the outgoing-wave boundary condition for ϕ with arbitrary l at any time t, we consider the differential formula for spherical Hankel function (Abramowitz and Stegun 1965)

$$\left(\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^l [z^l g_l(z)] = \exp(\mathrm{i}z), \tag{3.8}$$

which readily leads to

$$\frac{1}{\omega^l}\left(\frac{1}{r}\partial_r\right)^l [r^l g_l(\omega r)\exp(-\mathrm{i}\omega t)] = \exp \mathrm{i}(\omega r - \omega t). \tag{3.9}$$

We note that the right-hand side of (3.9) vanishes upon the operation $r(\partial_r + \partial_t)$. Taking the outgoing wave condition (3.5) into consideration, we show from (3.9) an outgoing boundary condition in the time domain

$$\partial_r \left(\frac{1}{r}\partial_r\right)^l [r^l \phi(r, t)] + \left(\frac{1}{r}\partial_r\right)^l [r^l \hat{\phi}(r, t)] = 0, \tag{3.10}$$

which holds for arbitrary l at any time t. Explicit expressions of the outgoing boundary condition evaluated at $r = a^+$ for cases with $l = 1, 2$ are worked out and given respectively by

$$\phi - a\phi' - a\hat{\phi} - a^2\phi'' - a^2\hat{\phi}' = 0; \tag{3.11}$$

$$3\phi' - 3a\phi'' - 3a\hat{\phi}' - a^2\phi''' - a^2\hat{\phi}'' = 0. \tag{3.12}$$

3.3. Wave evolution

For outgoing waves that satisfy the above-mentioned conditions we can evolve the field inside the system solely in terms of relevant QNMs. We will show this by considering the solution of the three-dimensional time-dependent wave equation (2.6), which can be expressed as an integral along a closed loop on the r–t plane:

$$\begin{aligned}\phi(r, t) = &\int_0^{a^+} \mathrm{d}r' \rho(r')\epsilon(r')[\phi(r', t')\partial_{t'} G(r, r'; t - t') - G(r, r'; t - t')\partial_{t'}\phi(r', t')]_{t'=0}^{t'=\infty} \\ &- \int_0^t \mathrm{d}t' \rho(r')[\phi(r', t')\partial_{r'} G(r, r'; t - t') - G(r, r'; t - t')\partial_{r'}\phi(r', t')]_{r'=0}^{r'=a^+},\end{aligned} \tag{3.13}$$

which is merely a direct generalization of the usual Green's theorem. In the first integral, the integrand vanishes along the line $t' = \infty$ by virtue of the causal initial condition $G(r, r'; t - t') = 0$ for $t \leqslant t'$. In the second integral, the integrand also vanishes at the lower limit since both ϕ and G vanish at the origin. Together with the fact that $\partial_{t'} G(r, r', t - t') = -\partial_t G(r, r', t - t')$, we have for $r \in [0, a]$ and $t > 0$,

$$\phi(r, t) = \int_0^{a^+} \mathrm{d}r'[\rho(r')\epsilon(r')\partial_t G(r, r'; t)\varphi(r') + G(r, r'; t)\hat{\varphi}(r')] + M(r, a^+; t), \tag{3.14}$$

where

$$M(r, r'; t) = \rho(r') \int_0^t \mathrm{d}t'[G(r, r'; t - t')\partial_{r'}\phi(r', t') - \partial_{r'} G(r, r'; t - t')\phi(r', t')]. \tag{3.15}$$

As a consequence, the wave field inside the system at a time t is completely determined by the initial data inside the system and a surface term that depends on the history of the wave at $r = a^+$.

Next, we show that the second integral in equation (3.14) can be written as a surface term by using the outgoing wave condition. For $r' > a$, ϕ and G can be written as

$$\phi(r', t') = \int d\omega_1 \mathcal{A}(\omega_1) g(\omega_1 r') \exp(-i\omega_1 t'), \tag{3.16}$$

$$G(r, r'; t - t') = \int d\omega_2\, \mathcal{B}(\omega_2, r) g(\omega_2 r') \exp[-i\omega_2(t - t')] \tag{3.17}$$

with some $\mathcal{A}$ and $\mathcal{B}$. Using equations (3.16) and (3.17), we have

$$\int_0^t dt' \rho(r') G(r, r'; t - t') \partial_{r'} \phi(r', t') = \rho(r') \int\int d\omega_1\, d\omega_2 \mathcal{A}(\omega_1) \mathcal{B}(\omega_2, r) \times [\partial_{r'} g(\omega_1 r')] g(\omega_2 r') \frac{\exp(-i\omega_2 t) - \exp(-i\omega_1 t)}{i(\omega_1 - \omega_2)}, \tag{3.18}$$

and, similarly,

$$\int_0^t dt' \rho(r') \partial_{r'} G(r, r'; t - t') \phi(r', t') = \rho(r') \int\int d\omega_1\, d\omega_2 \mathcal{A}(\omega_1) \mathcal{B}(\omega_2, r) \times g(\omega_1 r') [\partial_{r'} g(\omega_2 r')] \frac{\exp(-i\omega_2 t) - \exp(-i\omega_1 t)}{i(\omega_1 - \omega_2)}. \tag{3.19}$$

By virtue of these two equations, we show that

$$M(r, r'; t) = \int\int d\omega_1\, d\omega_2 \mathcal{A}(\omega_1) \mathcal{B}(\omega_2, r) [T(\omega_1, \omega_2; r', 0, t) - T(\omega_1, \omega_2; r', t, 0)], \tag{3.20}$$

where

$$T(\omega_1, \omega_2; r', t_1, t_2) \equiv \rho(r') \exp(-i\omega_1 t_1) \exp(-i\omega_2 t_2) \times \frac{[\partial_{r'} g(\omega_1 r')] g(\omega_2 r') - g(\omega_1 r') [\partial_{r'} g(\omega_2 r')]}{i(\omega_1 - \omega_2)}. \tag{3.21}$$

On the other hand, since $g(z)$ can be written as (Abramowitz and Stegun 1965)

$$g(z) = z h_l^{(1)}(z) = \sum_{k=0}^{l} \alpha_{lk} \frac{e^{iz}}{z^k}, \tag{3.22}$$

where

$$\alpha_{lk} \equiv i^{-l-1} \frac{(l + k)!}{k!(l - k)!} (-2i)^{-k}, \tag{3.23}$$

we find that T is given by

$$T = \sum_{k_1=1}^{l} \sum_{k_2=0}^{k_1-1} \sum_{n=0}^{k_1-k_2-1} i(k_2 - k_1) \alpha_{lk_1} \alpha_{lk_2} \frac{e^{i\omega_1(r'-t_1)}}{(\omega_1 r')^{k_2+1+n}} \frac{e^{i\omega_2(r'-t_2)}}{(\omega_2 r')^{k_1-n}} + [g(\omega_1 r')\, e^{-i\omega_1 t_1}][g(\omega_2 r')\, e^{-i\omega_2 t_2}]. \tag{3.24}$$

We further rearrange the first term in (3.24) and define A_{mn} such that

$$\sum_{m,n=1}^{l} \frac{e^{i\omega_1(r'-t_1)}}{(\omega_1 r')^m} A_{mn} \frac{e^{i\omega_2(r'-t_2)}}{(\omega_2 r')^n} \equiv \sum_{k_1=1}^{l} \sum_{k_2=0}^{k_1-1} \sum_{n=0}^{k_1-k_2-1} i(k_2 - k_1) \alpha_{lk_1} \alpha_{lk_2} \frac{e^{i\omega_1(r'-t_1)}}{(\omega_1 r')^{k_2+1+n}} \frac{e^{i\omega_2(r'-t_2)}}{(\omega_2 r')^{k_1-n}}. \tag{3.25}$$

Our immediate task is to express T in terms of $g(\omega_1 r')$, $g(\omega_2 r')$ and their derivatives. To this end, we introduce the operator $\hat{D}$:

$$\hat{D} \equiv r'(\partial_{r'} + \partial_t), \tag{3.26}$$

and it is then readily shown that

$$\hat{D}\left[\frac{\mathrm{e}^{\mathrm{i}\omega(r'-t)}}{(\omega r')^n}\right] = -n\left[\frac{\mathrm{e}^{\mathrm{i}\omega(r'-t)}}{(\omega r')^n}\right]. \tag{3.27}$$

Hence, by operating $\hat{D}$ on $[g(\omega r')\,\mathrm{e}^{-\mathrm{i}\omega t}]$, l times, we obtain a set of l equations:

$$\hat{D}^j[g(\omega r')\,\mathrm{e}^{-\mathrm{i}\omega t}] = \sum_{k=1}^{l} B_{jk}\frac{\mathrm{e}^{\mathrm{i}\omega(r'-t)}}{(\omega r')^k}, \qquad j = 1, \ldots, l, \tag{3.28}$$

where $\mathbf{B}$ is given by

$$\mathbf{B} = \begin{pmatrix} (-1)\alpha_{l1} & (-2)\alpha_{l2} & \ldots & (-l)\alpha_{ll} \\ (-1)^2\alpha_{l1} & (-2)^2\alpha_{l2} & \ldots & (-l)^2\alpha_{ll} \\ \vdots & \vdots & \ddots & \vdots \\ (-1)^l\alpha_{l1} & (-2)^l\alpha_{l2} & \ldots & (-l)^l\alpha_{ll} \end{pmatrix}. \tag{3.29}$$

Note that

$$\begin{aligned} \det\mathbf{B} &= (-1)^{l(l+1)/2}\prod_{k=1}^{l}\alpha_{lk}\det\begin{pmatrix} 1 & 2 & \ldots & l \\ 1^2 & 2^2 & \ldots & l^2 \\ \vdots & \vdots & \ddots & \vdots \\ 1^l & 2^l & \ldots & l^l \end{pmatrix} \\ &= (-1)^{l(l+1)/2}\prod_{k=1}^{l}\alpha_{lk}\prod_{j=1}^{l} j\prod_{k=1}^{j-1}(j-k) \neq 0. \end{aligned} \tag{3.30}$$

To arrive at the second line, we have used the formula for Vandermonde's determinant (Lang 1986). Thus $\mathbf{B}$ is always nonsingular and we can invert equation (3.28) to obtain

$$\frac{\mathrm{e}^{\mathrm{i}\omega(r'-t)}}{(\omega r')^j} = \sum_{k=1}^{l} B^{-1}_{jk}\hat{D}^k[g(\omega r')\,\mathrm{e}^{-\mathrm{i}\omega t}], \qquad j = 1, \ldots, l. \tag{3.31}$$

With this expression, equation (3.24) can be rewritten as

$$T = \sum_{m,n=0}^{l} \hat{D}_1^m[g(\omega_1 r')\,\mathrm{e}^{\mathrm{i}\omega_1 t_1}]M_{mn}\hat{D}_2^n[g(\omega_2 r')\,\mathrm{e}^{\mathrm{i}\omega_2 t_2}], \tag{3.32}$$

where $\hat{D}_{1,2} \equiv r'(\partial_{r'} + \partial_{t_{1,2}})$ and

$$M_{mn} = (1-\delta_{m0})(1-\delta_{n0})\sum_{j,k=1}^{l} A_{jk}B^{-1}_{jm}B^{-1}_{kn} + \delta_{m0}\delta_{n0}. \tag{3.33}$$

Putting it into equation (3.20), we have

$$M(r, a^+; t) = \sum_{m,n=0}^{l} \hat{D}_1'^m[G(r, r', t_1)]M_{mn}\hat{D}_2'^n[\phi(r', t_2)]|_{r'=a^+, t_1=t, t_2=0}. \tag{3.34}$$

It is obvious that equation (3.34) contains high-order time derivatives. However, since both ϕ and G satisfy the wave equation, we can replace $\partial_t^2\phi$ by $\left[\partial_r^2 - l(l+1)/r^2\right]\phi$. Repeated use of this replacement enables us to eliminate all second (or higher) order t-derivatives.

To sum up, we have obtained the following evolution formula:

$$\phi(r,t) = \int_0^{a^+} \mathrm{d}r'[G(r,r';t)\hat{\varphi}(r') + \rho(r')\epsilon(r')\partial_t G(r,r';t)\varphi(r')] + S(G,\varphi), \tag{3.35}$$

where the surface term is given by

$$S(G,\varphi) \equiv \mathbf{G}_l^T \mathbf{S}_l \Phi_l, \tag{3.36}$$

which is a bilinear form of $(\varphi, \hat{\varphi})$ and $(G, \partial_t G)$ and their r derivatives and can be expressed as a product of three matrices, namely the transpose of $\mathbf{G}_l$, $\mathbf{S}_l$ and Φ_l. While $\mathbf{S}_l$ is an $(l+1)\times(l+1)$ constant matrix, $\mathbf{G}_l$ and Φ_l are $(l+1)\times 1$ matrices which are respectively derivable from $(\varphi, \hat{\varphi})$ and $(G, \partial_t G)$. Explicit expressions for these matrices are given below for cases $l = 1, 2$:

$$\mathbf{G}_1 = \begin{pmatrix} G(r,a;t) \\ a[\partial_{r'}G(r,r'=a;t) + \partial_t G(r,a,;t)] \end{pmatrix}, \tag{3.37}$$

$$\mathbf{S}_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.38}$$

and

$$\Phi_1 = \begin{pmatrix} \varphi(a) \\ a[\partial_{r'}\varphi(r'=a) + \hat{\varphi}(a)] \end{pmatrix}, \tag{3.39}$$

$$\mathbf{G}_2 = \begin{pmatrix} G(r,a;t) \\ a[\partial_{r'}G(r,r'=a;t) + \partial_t G(r,a;t)] \\ a^2\left[\partial_{r'}^2 G(r,r'=a;t) + \partial_{r'}\partial_t G(r,r'=a;t)\right] \end{pmatrix}, \tag{3.40}$$

$$\mathbf{S}_2 = \frac{1}{3}\begin{pmatrix} 12 & -3 & -3 \\ -3 & 0 & 1 \\ -3 & 1 & 0 \end{pmatrix} \tag{3.41}$$

and

$$\Phi_2 = \begin{pmatrix} \varphi(a) \\ a[\partial_{r'}\varphi(r'=a) + \hat{\varphi}(a)] \\ a^2\left[\partial_{r'}^2\varphi(r'=a) + \partial_{r'}\hat{\varphi}(r'=a)\right] \end{pmatrix}. \tag{3.42}$$

For convenience we have used a to indicate a^+ in these formulae.

3.4. Two-component expansion

The formula in (3.35) implies that the evolution of $\phi(r,t)$ inside the cavity is independent of the initial data outside the cavity, whose effect is represented by the surface term. In particular, we can now derive the two-component expansion with this evolution formula. Inserting the QNM expansion of the Green's function (2.11) into (3.35), we then obtain

$$\begin{pmatrix} \phi(r,t) \\ \hat{\phi}(r,t) \end{pmatrix} = \sum_j a_j \begin{pmatrix} 1 \\ -\mathrm{i}\omega_j\rho(r)\epsilon(r) \end{pmatrix} f_j(r)\,\mathrm{e}^{-\mathrm{i}\omega_j t}, \tag{3.43}$$

for $r \in [0, a]$, where a_j is given by the projection formula

$$a_j = \frac{\mathrm{i}}{2\omega_j}\left\{\int_0^{a^+} \mathrm{d}r'[f_j(r')\hat{\varphi}(r') + \hat{f}_j(r')\varphi(r')] + S(f_j e^{-\mathrm{i}\omega_j t}, \varphi)|_{t=0}\right\}. \tag{3.44}$$

Here we have introduced $\hat{f}_j = -\mathrm{i}\omega_j \rho\epsilon f_j$. By taking $t \to 0^+$ in (3.43) one obtains the two-component expansion (3.1). The projection formula is exactly the same as that for the one-dimensional case, except that the definition of the surface term has been modified. Note that for $l = 0$, $g(\omega r) \propto \mathrm{e}^{\mathrm{i}\omega r}$ for $r > a$. The surface term becomes $S = f_j(a)\varphi(a)$, and thus recovering the previous result.

4. Linear space structure

With the two-component expansion established, we develop here the associated linear space structure for outgoing waves. Most importantly, the time-evolution operator is shown to be self-adjoint. It then leads to all the results exactly the same as those in the one-dimensional case, except that the definition of the surface term in the inner product has to be modified.

Consider the function space of outgoing waves Γ, denoted as $|\phi\rangle = (\phi, \hat{\phi})^T$. The corresponding eigenbra is then denoted as $\langle\phi| = (\hat{\phi}, \phi)$. The wave equation can be recast in the time-dependent Schrödinger form

$$\frac{\partial}{\partial t}|\phi\rangle = -\mathrm{i}\mathcal{H}|\phi\rangle, \tag{4.1}$$

where

$$\mathcal{H} = \mathrm{i}\begin{pmatrix} 0 & (\rho\epsilon)^{-1} \\ \hat{L}_l & 0 \end{pmatrix}, \tag{4.2}$$

with the operator $\hat{L}_l$ defined as

$$\hat{L}_l \equiv \frac{\partial}{\partial r}\rho(r)\frac{\partial}{\partial r} - \rho(r)\frac{l(l+1)}{r^2}. \tag{4.3}$$

For any two vectors $|\phi\rangle$ and $|\psi\rangle$ belonging to Γ, we define the generalized inner product as

$$\langle\psi|\phi\rangle = \mathrm{i}\left\{\int_0^{a^+} \mathrm{d}r[\hat{\psi}(r)\phi(r) + \psi(r)\hat{\phi}(r)] + S(\psi,\phi)\right\}. \tag{4.4}$$

With the generalized inner product (4.4), the projection formula (3.44) can be written compactly as

$$a_j = \frac{\langle f_j|\phi\rangle}{\langle f_j|f_j\rangle} = \frac{1}{2\omega_j}\langle f_j|\phi\rangle. \tag{4.5}$$

Despite that the surface term S, in general, is quite complicated for large l, for any two different QNMs, the surface term is simply

$$S(f_n, f_p) = \rho\left.\frac{f_n' f_p - f_n f_p'}{\mathrm{i}(\omega_n - \omega_p)}\right|_{r=a^+}. \tag{4.6}$$

This can be obtained by putting $\mathcal{A} = \delta(\omega - \omega_n)$ and $\mathcal{B} = \delta(\omega - \omega_p)$ in equation (3.20).

Alternatively, the generalized inner product (4.4) and the explicit form of the surface term (4.6) can be readily derived in the time-independent context. The QNMs are defined by

$$\left[-\frac{\mathrm{d}}{\mathrm{d}r}\rho(r)\frac{\mathrm{d}}{\mathrm{d}r} + \rho(r)\frac{l(l+1)}{r^2} - \rho(r)\epsilon(r)\omega_n^2\right] f_n(r) = 0. \tag{4.7}$$

Consider two distinct QNMs, $f_n(r)$ and $f_p(r)$. Start with their defining equations and usual manipulations lead to

$$\int_0^{a^+} \mathrm{d}r\left(-f_p\frac{\mathrm{d}}{\mathrm{d}r}\rho\frac{d}{dr}f_n + f_n\frac{\mathrm{d}}{\mathrm{d}r}\rho\frac{\mathrm{d}}{\mathrm{d}r}f_p\right) - \int_0^{a^+} \mathrm{d}r\ \rho\epsilon\left(\omega_n^2 - \omega_p^2\right) f_n f_p = 0. \tag{4.8}$$

Then we can obtain the orthogonality relation

$$\int_0^{a^+} \mathrm{d}r\ \rho\epsilon f_n f_p + \left.\frac{f_n' f_p - f_n f_p'}{\omega_n^2 - \omega_p^2}\right|_{r=a^+} = 0, \tag{4.9}$$

where $' \equiv \partial_r$. Since $\hat{f}_n = -\mathrm{i}\omega_n \rho\epsilon f_n$, from equation (4.9) we have

$$\int_0^{a^+} \mathrm{d}r(f_n\hat{f}_p + \hat{f}_n f_p) + \left.\frac{f_n' f_p - f_n f_p'}{\mathrm{i}(\omega_n - \omega_p)}\right|_{r=a^+} = 0. \tag{4.10}$$

We then show the two-component orthogonality relation for QNMs, namely $\langle f_i|f_j\rangle = 2\omega_j\delta_{ij}$.

We now go back to check whether the time-evolution operator $\mathcal{H}$ is a self-adjoint operator under the generalized inner product, namely

$$\langle\psi|\{\mathcal{H}|\phi\rangle\} = \langle\phi|\{\mathcal{H}|\psi\rangle\}. \tag{4.11}$$

The matrix element $\langle\psi|\{\mathcal{H}|\phi\rangle\}$ is given by equation (4.4) with $\mathcal{H}|\phi\rangle$ in place of $|\phi\rangle$, i.e.

$$\begin{pmatrix}\phi\\ \hat{\phi}\end{pmatrix} \mapsto \begin{pmatrix}\mathrm{i}(\rho\epsilon)^{-1}\hat{\phi}\\ \mathrm{i}\hat{L}_l\phi\end{pmatrix}. \tag{4.12}$$

Hence,

$$\langle\psi|\{\mathcal{H}|\phi\rangle\} = -\int_0^{a^+} \mathrm{d}r[\psi(\partial_r\rho\partial_r - \rho l(l+1)/r^2)\phi + \hat{\psi}\hat{\phi}] + \mathrm{i}S(\psi, \mathcal{H}\phi). \tag{4.13}$$

Integrating the first term in equation (4.13) by parts twice, we have

$$\langle\psi|\{\mathcal{H}|\phi\rangle\} = -\int_0^{a^+} \mathrm{d}r[\phi(\partial_r\rho\partial_r - \rho l(l+1)/r^2)\psi + \hat{\psi}\hat{\phi}] - \psi\phi' + \psi'\phi|_{r=a^+} + \mathrm{i}S(\psi, \mathcal{H}\phi). \tag{4.14}$$

For $r \geqslant a$, ψ and ϕ satisfy the outgoing-wave boundary condition

$$\phi(r,t) = \int \mathrm{d}\omega_1\, \mathcal{A}_1(\omega_1) g(\omega_1 r)\, \mathrm{e}^{-\mathrm{i}\omega_1 t}, \tag{4.15}$$

$$\psi(r,t) = \int \mathrm{d}\omega_2\, \mathcal{A}_2(\omega_1) g(\omega_2 r)\, \mathrm{e}^{-\mathrm{i}\omega_2 t}, \tag{4.16}$$

for some suitable $\mathcal{A}_1$ and $\mathcal{A}_2$. Hence

$$-\psi\phi' + \psi'\phi|_{r=a^+} = \int\int \mathrm{d}\omega_1\, \mathrm{d}\omega_2\, \mathcal{A}_1(\omega_1)\mathcal{A}_2(\omega_2)[-g(\omega_2 r)g'(\omega_1 r) + g'(\omega_2 r)g(\omega_1 r)]_{r=a^+}. \tag{4.17}$$

Substituting equation (4.15) into equation (4.12), we have

$$\mathcal{H}|\phi\rangle = \begin{pmatrix}\int \mathrm{d}\omega_1[\omega_1\mathcal{A}_1(\omega_1)]g(\omega_1 r)\,\mathrm{e}^{-\mathrm{i}\omega_1 t}\\ \int \mathrm{d}\omega_1[\omega_1\mathcal{A}_1(\omega_1)]\hat{g}(\omega_1 r)\,\mathrm{e}^{-\mathrm{i}\omega_2 t}\end{pmatrix}, \tag{4.18}$$

where we have used the wave equation and $\hat{g}(\omega_1 r) = -\mathrm{i}\omega_1 g(\omega_1 r)$. In other words, the effect of $\mathcal{H}$ on $|\phi\rangle$ amounts to the replacement $\mathcal{A}_1(\omega_1) \mapsto \omega_1\mathcal{A}_1(\omega_1)$. Hence

$$\mathrm{i}S(\psi, \mathcal{H}\phi) = \int\int \mathrm{d}\omega_1\, \mathrm{d}\omega_2\omega_1\, \mathcal{A}_1(\omega_1)\mathcal{A}_2(\omega_2)\left.\frac{g'(\omega_2 r)g(\omega_1 r) - g(\omega_2 r)g'(\omega_1 r)}{\omega_2 - \omega_1}\right|_{r=a^+}. \tag{4.19}$$

Adding equations (4.17) and (4.19), we have

$$
\begin{aligned}
-\psi\phi' + \psi'\phi|_{r=a^+} + \mathrm{i}S(\psi, \mathcal{H}\phi) &= \int\int \mathrm{d}\omega_1\,\mathrm{d}\omega_2 \left[1 + \frac{\omega_1}{\omega_2 - \omega_1}\right] \mathcal{A}_1(\omega_1)\mathcal{A}_2(\omega_2) \\
&\quad \times [g'(\omega_2 r)g(\omega_1 r) - g(\omega_2 r)g'(\omega_1 r)]|_{r=a^+} \\
&= \int\int \mathrm{d}\omega_1\,\mathrm{d}\omega_2 \mathcal{A}_1(\omega_1)[\omega_2\mathcal{A}_2(\omega_2)] \left.\frac{g'(\omega_1 r)g(\omega_2 r) - g(\omega_1 r)g'(\omega_2 r)}{\omega_1 - \omega_2}\right|_{r=a^+} \\
&= \mathrm{i}S(\phi, \mathcal{H}\psi).
\end{aligned} \tag{4.20}
$$

Putting equation (4.20) into equation (4.14), we have

$$
\begin{aligned}
\langle\psi|\{\mathcal{H}|\phi\rangle\} &= -\int_0^{a^+} \mathrm{d}r[\phi(\partial_r\rho\partial_r - l(l+1)/r^2)\psi + \hat{\psi}\hat{\phi}] + \mathrm{i}S(\phi, \mathcal{H}\psi) \\
&= \langle\phi|\{\mathcal{H}|\psi\rangle\},
\end{aligned} \tag{4.21}
$$

showing that $\mathcal{H}$ is self-adjoint. This in turn establishes the orthogonality relation between any two non-degenerate eigenvectors of $\mathcal{H}$, which then completes our development of the two-component formalism for waves in open spherical cavities.

5. Time-dependent wave evolution

Having developed the two-component formalism for waves in open spherical cavities and generalized the outgoing-wave boundary condition to the case with a centrifugal barrier, we remark that the outgoing-wave boundary condition has an immediate application in the evolution of outgoing waves. This condition allows the waves to pass through the computational domain without spurious reflections. In other words, the evolution problem in an infinite domain can be replaced by a problem in a finite domain with the outgoing-wave boundary condition imposed at the surface of the system.

In fact, the construction of an outgoing-wave boundary condition is a challenge common to various problems related to numerical solution of wave propagation in infinite domain and has been an active area of research. Closely related to our problem is the work of Grote and Keller (1995). They have derived an exact non-reflecting boundary condition (NRBC) for solutions of the time-dependent wave equation in three space dimensions. Then they combined the NRBC with finite differencing methods and finite element methods, and presented some numerical examples which demonstrate the high accuracy of their NRBC (Grote and Keller 1996). Recently, they extended these ideas to the electromagnetic wave scattering (Grote and Keller 1998) and elastic wave scattering (Grote and Keller 2000).

Similarly, with the two-component formulation, one can evolve $\phi(r, t)$ in the finite domain $0 \leqslant r \leqslant a$ with the outgoing-wave boundary condition at the surface $r = a^+$, under the given initial conditions $\varphi(r)$ and $\hat{\varphi}(r)$. The wavefunctions $\phi(r, t)$ and $\partial_t\phi(r, t)$ are expanded by two-component QNMs as shown in equations (3.43) and (3.44); hence, time-dependent wave evolution can be obtained. Numerical results demonstrating the validity of the formulation and the boundary condition will be presented in the next section.

6. Numerical examples

This section presents some numerical examples to put the discussion into context, and to illustrate the two-component QNM eigenfunction expansion. As an example, consider a uniform dielectric sphere of radius a with dielectric constant distribution given by

$\epsilon(r) = 1 + \left(n_{\mathrm{I}}^2 - 1\right)\theta(a - r)$. By matching the boundary conditions at $r = a$, it is readily shown that the eigenfrequencies ω are obtained by the solutions of the following equation:

$$\rho \frac{\mathrm{d}[r j_l(n_{\mathrm{I}}\omega r)]}{\mathrm{d}r}\bigg|_{r=a} = \frac{j_l(n_{\mathrm{I}}\omega a)}{h_l^{(1)}(\omega a)} \frac{\mathrm{d}\left[r h_l^{(1)}(\omega r)\right]}{\mathrm{d}r}\bigg|_{r=a}, \tag{6.1}$$

where j_l and $h_l^{(1)}$ are the spherical Bessel and Hankel functions. The normalized QNM eigenfunctions are defined as

$$f_j(r) = \begin{cases} r j_l(n_{\mathrm{I}}\omega_j r)/N_{\nu jl}, & \text{for} \quad 0 \leqslant r \leqslant a \\ \left[j_l(n_{\mathrm{I}}x_j)\big/h_l^{(1)}(x_j)\right] r h_l^{(1)}(\omega r)/N_{\nu jl}, & \text{for} \quad r > a, \end{cases} \tag{6.2}$$

where $x_j = \omega_j a$, and the norm $N_{\nu jl}^2$ for the TE and TM modes are, respectively, given by

$$N_{1jl}^2 = \left(n_{\mathrm{I}}^2 - 1\right)\frac{a^3}{2} j_l^2(n_{\mathrm{I}}x_j) \tag{6.3}$$

and

$$N_{2jl}^2 = \left(1 - \frac{1}{n_{\mathrm{I}}^2}\right)\left\{\left[\frac{j_l'(n_{\mathrm{I}}x_j)}{j_l(n_{\mathrm{I}}x_j)} + \frac{1}{n_{\mathrm{I}}x_j}\right]^2 + \frac{l^2 + l}{x_j^2}\right\}\frac{a^3}{2} j_l^2(n_{\mathrm{I}}x_j). \tag{6.4}$$

One may show that the eigenfunction f_j satisfies the orthogonality relation (2.10), namely $\langle f_i | f_j \rangle = 2\omega_j \delta_{ij}$. In addition, both f_j and $\rho f_j'$ are continuous at $r = a$.

6.1. Validity of two-component expansion

As an example to demonstrate the expansion of two-component waves, we consider $\varphi(r) = (r/a)^4$ for $0 \leqslant r \leqslant a$, and for $r > a, \varphi(r)$ is equal to $(r/a)^4$ and $(r/a)^{4/n_{\mathrm{I}}^2}$ for TE and TM QNM expansions, respectively. This choice of φ can ensure that the boundary conditions for the electric and magnetic fields across the surface of the dielectric sphere are satisfied. On the other hand, we let $\hat{\varphi}(r) = K\rho(r)\epsilon(r)(r/a)^3 \exp(-qr/a)$, or equivalently $\partial_t \phi(r, t = 0) = K(r/a)^3 \exp(-qr/a)$, where q is an arbitrary constant and K is determined by the outgoing wave condition. For such a choice of φ and $\hat{\varphi}$, the expansion coefficients a_j could then been obtained analytically from the projection formula (3.44).

To gauge the rate of convergence of the two-component expansion, we evaluated the partial sums on the right-hand side of (3.1) up to $|j| \leqslant N$, and considered the root-mean-square deviations from the exact values of φ and $\hat{\varphi}$, which are respectively defined as

$$\Delta_1(N) = \sqrt{\frac{1}{a}\int^{a^-} \left|\sum_{|j|\leqslant N} a_j f_j(r) - \varphi(r)\right|^2 \mathrm{d}r} \tag{6.5}$$

$$\Delta_2(N) = \sqrt{\frac{1}{a}\int^{a^-} \left|-\mathrm{i}\omega_j \rho\epsilon \sum_{|j|\leqslant N} a_j f_j(r) - \hat{\varphi}(r)\right|^2 \mathrm{d}r}. \tag{6.6}$$

Figures 1 and 2 show the deviations for the cases $l = 1$ and $l = 2$, respectively. It can be shown that $\Delta_1(N)$ and $\Delta_2(N)$ roughly go as N^{-3} and N^{-2}, respectively.

The two-component expansion proposed here properly takes the outgoing boundary condition into consideration. Therefore, unlike conventional Fourier series expansion that usually imposes an artificial nodal boundary condition at the boundary, the two-component expansion is valid at the boundary of the open system. To investigate the convergence rate at

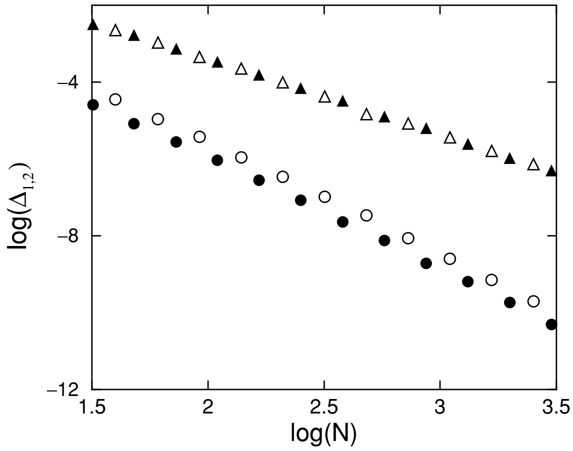

Figure 1. The solid (empty) circles and triangles represent, respectively, $\Delta_1(N)$ ($\Delta_2(N)$) using TE (TM) QNM expansion with $l = 1$. Here $q = 1.7$.

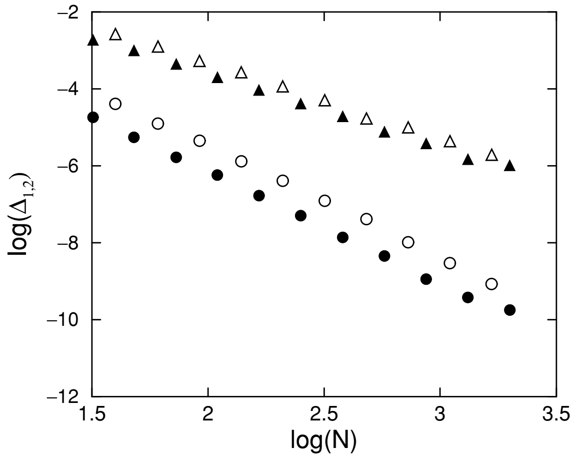

Figure 2. Same as figure 1, except for $l = 2$.

$r = a$, we define

$$\Delta_3(N) = \left|\sum_j^N a_j f_j(a) - \varphi(a)\right|, \tag{6.7}$$

$$\Delta_4(N) = \left|-\mathrm{i}\omega_j \rho\epsilon \sum_j^N a_j f_j(a) - \hat{\varphi}(a)\right| \tag{6.8}$$

and show them as functions of N in figure 3 (figure 4) for $l = 1$ ($l = 2$). It is obvious that both expansions converge to the correct values, and the deviations $\Delta_3(N)$ and $\Delta_4(N)$ are proportional to N^{-3} and N^{-1}, respectively.

It is worthwhile to make use of this numerical example to illustrate the significance of the surface term appearing in the projection formula (3.44). As mentioned above, we considered

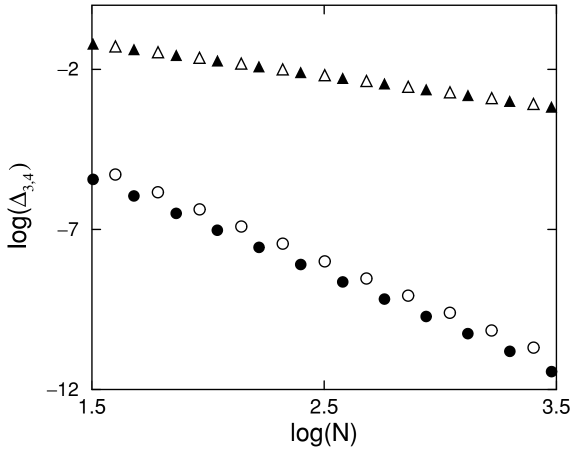

Figure 3. The solid (empty) circles and triangles represent, respectively, $\Delta_3(N)$ ($\Delta_4(N)$) using TE (TM) QNM expansion with $l = 1$. Here $q = 1.7$.

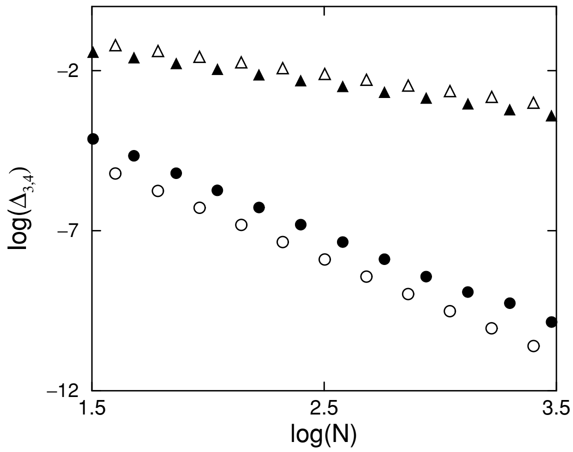

Figure 4. Same as figure 4, except for $l = 2$.

φ and $\hat{\varphi}$ that satisfy the outgoing wave condition for $l = 2$. However, we deliberately used the surface term for $l = 1$ to calculate the expansion coefficients a_j. In this case we found that (i) the partial sum for φ still converges to the correct value with $\Delta_1 \sim N^{-2}$ and $\Delta_3 \sim N^{-1}$ and (ii) the partial sum for $\hat{\varphi}$ converges to the correct value with $\Delta_2 \sim N^{-1}$, but it does not converge to the correct value at $r = a$. Thus, the two-component formalism provides an effective method to expand a pair of functions $(\varphi, \hat{\varphi})$ satisfying the outgoing boundary condition in terms of rapidly convergent QNMs series.

6.2. Wave evolution in two-component expansion

As discussed above, equation (3.43) directly leads to a simple solution to the evolution of waves inside a open cavity. To examine the validity and accuracy of this method, we consider the following initial conditions:

$$\varphi(r) = r^2(a - r)^2, \tag{6.9}$$

$$\hat{\varphi}(r) = 0, \tag{6.10}$$

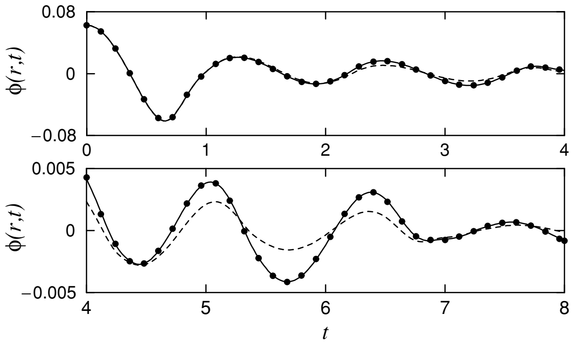

Figure 5. The figure depicts $\phi(r = a/2, t)$ as a function of t (in units of a) for the TE case with $l = 2$ under the initial conditions given by (6.9) and (6.10). The results obtained from the TE two-component expansion (solid circles) show good agreement with those from the numerical solution with $\Lambda = 5a$ (continuous line). For purpose of comparison, the numerical results with $\Lambda = 1.01a$ (dashed line) are also shown.

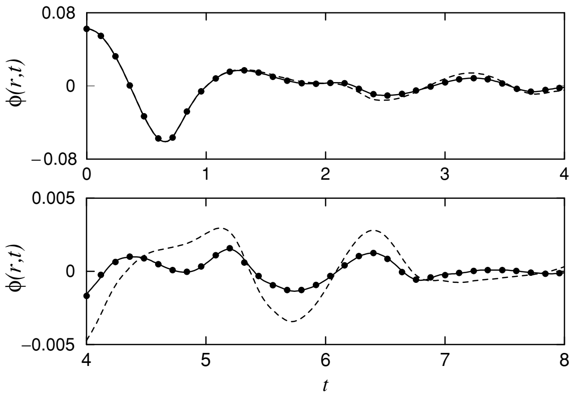

Figure 6. Same as figure 5, except that the wave is governed by the TM wave equation and TM QNMs are used to expand the wave field.

for $0 \leqslant r \leqslant a$ and $\varphi(r) = \hat{\varphi}(r) = 0$ otherwise. Such initial condition represents a wave initially confined in the dielectric sphere. It is obvious that both the regular boundary condition at $r = 0$ and outgoing-wave boundary condition at $r = a$ are satisfied. The wavefunctions $\phi(r, t)$ and $\partial_t\phi(r, t)$ for $t > 0$ are then obtained from (3.43) and (3.44). In order to provide a benchmark for comparison, we also numerically solve the wave equation in the finite interval $0 \leqslant r \leqslant \Lambda$ and impose the standard Sommerfeld radiation boundary condition $(\partial_r + \partial_t)\phi(r, t) = 0$ at $r = \Lambda$. Although this condition is a great improvement over the nodal boundary condition, it could still give rise to spurious reflections at the computational boundary $r = \Lambda$ (see, e.g. Agudin and Platzeck (1974)). However, it is well known that such numerical scheme is accurate if $\Lambda \gg a$.

Figures 5 and 6 depict the temporal evolution of $\phi(r = a/2, t)$ governed by the TE and TM wave equations respectively for the case $l = 2$. The results obtained from the two-component expansion (solid circles) show good agreement with those of the numerical solution for the case $\Lambda = 5a$ (continuous line). Here we have retained QNMs with $|j| \leqslant 50$. For purpose of comparison, the numerical results with $\Lambda = 1.01a$ (dashed line) are also shown in figures 5 and 6. It is obvious that for sufficiently long time the two-component time-dependent expansion indeed outperforms numerical schemes that impose the Sommerfeld radiation boundary condition just outside the dielectric sphere.

7. Time-independent perturbation theory

With the completeness and orthogonality of the two-component eigenfunctions as discussed above, we can also derive a time-independent perturbation theory for QNMs. As a concrete example, we consider a reference system with a radius a and a dielectric constant distribution $\epsilon^{(0)}(r)$ and assume that the complete set of QNMs of this system are known. The pth QNM of the unperturbed system, which has an eigenfrequency $\omega_p^{(0)}$ and eigenfunction $f_p^{(0)}$, is defined by the eigenvalue equation

$$\mathcal{H}_0 \big| f_p^{(0)} \big\rangle = \omega_p^{(0)} \big| f_p^{(0)} \big\rangle, \tag{7.1}$$

where

$$\mathcal{H}_0 = \mathrm{i} \begin{pmatrix} 0 & (\rho^{(0)}\epsilon^{(0)})^{-1} \\ \partial_r \rho^{(0)} \partial_r - \rho^{(0)} l(l+1)/r^2 & 0 \end{pmatrix}. \tag{7.2}$$

We now switch our attention to another system—the perturbed system—which is described by a dielectric constant $\epsilon(r) = \epsilon^{(0)}(r) + \delta\epsilon(r)$ and, accordingly, $\rho(r) = \rho^{(0)}(r) + \delta\rho(r)$. The perturbation $\delta\epsilon(r)$ is assumed to be nonzero only inside the system, i.e. $r \leqslant a$. The corresponding eigenvalue equation for the perturbed system is

$$\mathcal{H}|f_p\rangle = \omega_p |f_p\rangle, \tag{7.3}$$

where

$$\mathcal{H} = \mathcal{H}_0 + \mu\mathcal{V} \tag{7.4}$$

and

$$\mathcal{V} = \mathrm{i} \begin{pmatrix} 0 & (\rho\epsilon)^{-1} - (\rho^{(0)}\epsilon^{(0)})^{-1} \\ \partial_r \delta\rho \partial_r - \delta\rho l(l+1)/r^2 & 0 \end{pmatrix}. \tag{7.5}$$

Here μ is merely a formal expansion parameter and will be set equal to unity after developing the perturbation series.

As usual we expand ω_p in powers of μ

$$\omega_p = \omega_p^{(0)} + \mu\omega_p^{(1)} + \mu^2\omega_p^{(2)} + \cdots. \tag{7.6}$$

By virtue of the completeness and orthogonality of the two-component eigenfunctions, one may derive the perturbative corrections $\omega_p^{(i)}$ $(i = 1, 2, \ldots)$ using the standard techniques in the Rayleigh–Schrödinger perturbation theory. The leading eigenfrequency shifts are then given by

$$\omega_p^{(1)} = \frac{\omega_p^{(0)}}{2} V_{pp}, \tag{7.7}$$

$$\omega_p^{(2)} = \frac{\omega_p^{(0)}}{4} \sum_{m \neq p} V_{pm} \frac{\omega_m^{(0)}}{\big[\omega_p^{(0)} - \omega_m^{(0)}\big]} V_{mp}, \tag{7.8}$$

$$\omega_p^{(3)} = \frac{\omega_p^{(0)}}{8} \left\{ \sum_{m \neq p} \sum_{q \neq p} V_{pm} \frac{\omega_m^{(0)}}{\big[\omega_p^{(0)} - \omega_m^{(0)}\big]} V_{mq} \frac{\omega_q^{(0)}}{\big[\omega_p^{(0)} - \omega_q^{(0)}\big]} V_{qp} - V_{pp} \sum_{m \neq p} V_{pm} \frac{\omega_m^{(0)}\omega_p^{(0)}}{\big[\omega_p^{(0)} - \omega_m^{(0)}\big]^2} V_{mp} \right\}. \tag{7.9}$$

Here the matrix elements are defined as

$$\langle f_p^{(0)} | \mathcal{V} | f_m^{(0)} \rangle \equiv \omega_p^{(0)} \omega_m^{(0)} V_{pm}, \tag{7.10}$$

where

$$V_{pm} = \int_0^a \mathrm{d}r\, f_p^{(0)} \epsilon^{(0)} [\epsilon^{(0)}/\epsilon - 1] f_m^{(0)} \tag{7.11}$$

for the TE modes, and

$$V_{pm} = \frac{1}{\omega_p^{(0)} \omega_m^{(0)}} \int_0^a \mathrm{d}r\, \delta\rho \left\{ \left[\frac{\mathrm{d}}{\mathrm{d}r} f_p^{(0)} \right] \left[\frac{\mathrm{d}}{\mathrm{d}r} f_m^{(0)} \right] + \frac{l(l+1)}{r^2} f_p^{(0)} f_m^{(0)} \right\} \tag{7.12}$$

for the TM modes. It is worthwhile to compare these formulae with the ones obtained by the Green's function method (Leung and Pang 1996). While the perturbative corrections obtained from the two methods are the same for the TM mode case, they are different for the TE mode case. The differences are rooted in the fact that now the perturbation is measured in $\delta(1/\epsilon) = \epsilon^{-1} - \epsilon_0^{-1}$, rather than $\delta\epsilon = \epsilon - \epsilon_0$ as in the previous method. In fact, one can show that both results become identical to each other if $\delta(1/\epsilon)$ is expanded in a power series of $\delta\epsilon$.

8. Conclusion

From a time-dependent view point, we develop a two-component formalism for QNMs, which properly solves the evolution problem of waves in open spherical systems. On the other hand, the two-component formalism also provides a natural and useful definition of inner product for QNMs and, in general, for any outgoing waves. In addition, we also show that the inner product in the two-component form leads to a linear space structure of outgoing waves, which resembles that of waves in closed systems. As a result, many familiar mathematical tools, e.g. time-independent perturbation method, can be developed in parallel with conservative systems. Thus, the two-component formalism developed here in fact put QNMs on a firm footing, on which various mathematical and computational analyses can thrive.

The completeness and orthogonality relations established here are valid for QNMs of spherically symmetric systems. However, with such relations we are well equipped to consider QNMs of asymmetric systems. For example, the QNM of an asymmetric system can be expanded as

$$|\phi\rangle = \sum_{lm,j} a_{lm,j} |f_{lm,j}\rangle, \tag{8.1}$$

where $|f_{lm,j}\rangle$ is the jth QNM of a spherical system and carries an angular momentum $\{lm\}$. In other words, $|f_{lm,j}\rangle$ is proportional to Y_{lm}. By orthogonality of $\{Y_{lm}\}$ and QNMs, it is easy to show that $\langle f_{l'm',j'} | f_{lm,j}\rangle \propto \delta_{ll'}\delta_{mm'}\delta_{jj'}$. Thus, perturbation expansion of QNMs of asymmetric systems can in principle be developed. Of course, detailed exposition of relevant theory is beyond the scope of the present paper and will be published elsewhere.

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