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Jordan blocks and generalized bi-orthogonal bases: realizations in open wave systems

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Abstract

Dissipation can sometimes be described by a non-Hermitian Hamiltonian H, whose left and right eigenvectors $\{\boldsymbol{f}^j, \boldsymbol{f}_j\}$ form a bi-orthogonal basis (BB). For waves in a class of open systems, this is known to lead to exact, complete BB expansions *if* $\langle \boldsymbol{f}^j | \boldsymbol{f}_j \rangle \neq 0$ for all j. If not, normalization seems impossible and many familiar formulae fail; examples are given. The problem is related to the merging of eigenmodes, so that H can only be diagonalized to Jordan blocks. The resolution involves a generalized BB containing extra vectors, whose dynamics are modified by polynomials in the time t. The splitting of merged modes under a perturbation is also treated. One thus obtains a non-trivial extension of the BB formalism for open systems.

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1. Introduction

For conservative, linear systems, governed by a Hermitian Hamiltonian, the crucial feature in their analysis is the existence of a complete spectrum. For spatially confined systems, the latter takes the form of a discrete set of orthogonal eigenfunctions. In terms of these, any function can be expanded by projection, effectively solving the time-evolution problem.

However, many physical systems, while still having their states in a Hilbert space with inner product $\langle \cdot | \cdot \rangle$, are naturally described by a *non-Hermitian Hamiltonian* (NHH) H [1]. At least in the finite-dimensional case, it then follows from the characteristic polynomial that the left ($H^\dagger \boldsymbol{f}^j = \omega_j^* \boldsymbol{f}^j$) and right ($H \boldsymbol{f}_j = \omega_j \boldsymbol{f}_j$) eigenvalues still coincide, but the corresponding eigenvectors need not. One may formalize the latter's 1–1 correspondence by introducing a duality map $\mathcal{D}\boldsymbol{f}_j = \boldsymbol{f}^j$, extended to the span of $\{\boldsymbol{f}_j\}$ by antilinearity $\mathcal{D}(\alpha\boldsymbol{\chi} + \beta\boldsymbol{\psi}) = \alpha^*\mathcal{D}\boldsymbol{\chi} + \beta^*\mathcal{D}\boldsymbol{\psi}$. Since $\mathcal{D}H\boldsymbol{f}_j = \omega_j^*\boldsymbol{f}^j = H^\dagger\mathcal{D}\boldsymbol{f}_j$, on that span one has

$$\mathcal{D}H = H^\dagger\mathcal{D}. \tag{1.1}$$

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Instead of the familiar orthogonality of eigenvectors one now has *bi-orthogonality* $\langle \boldsymbol{f}^j | \boldsymbol{f}_k \rangle = 0$, $j \neq k$ (we need only consider the case that all ω_j are different, cf section 3.1). *If* $\langle \boldsymbol{f}^j | \boldsymbol{f}_j \rangle \neq 0$ for all j and *if* (at least in some subspace) each vector ϕ has an expansion

$$\phi = \sum_j a_j \boldsymbol{f}_j \tag{1.2}$$

straightforward scalar multiplication leads to the projection formula

$$a_j = \frac{\langle \boldsymbol{f}^j | \phi \rangle}{\langle \boldsymbol{f}^j | \boldsymbol{f}_j \rangle}. \tag{1.3}$$

The $\{\boldsymbol{f}^j, \boldsymbol{f}_j\}$ are then said to constitute a *bi-orthogonal basis* (BB). BBs bring the advantages of a discrete eigenvector basis to non-Hermitian systems, establishing an analogy to their conservative counterparts. For instance, the dynamics are solved as

$$\mathrm{e}^{-\mathrm{i}Ht}\phi = \sum_j a_j \mathrm{e}^{-\mathrm{i}\omega_j t} \boldsymbol{f}_j \tag{1.4}$$

with a_j as in (1.3). As such, BBs are used in, e.g., cavity QED [2], chemical bonding [3], wavelets [4], and solid mechanics [5]. Since (1.4) describes damped behaviour if $\mathrm{Im}\,\omega_j < 0$, it is seemingly attractive to simply *postulate* an NHH as a model for dissipative systems.

Several complications can arise in the use of NHHs and BBs, cf the caveats above. *First*, especially in the infinite-dimensional case it is usually hard to establish completeness—the $\boldsymbol{f}_j$ may not span the whole (physically relevant sub-)space. In practice, completeness is often left as an assumption. *Second*, the reverse implication from (1.3) to (1.2) need not hold: instead of converging to a vector different from ϕ if completeness is violated, the sum over projections $\sum_j a_j \boldsymbol{f}_j$ may diverge altogether even for ϕ in the span of $\{\boldsymbol{f}_j\}$. Namely, without orthogonality the sum's norm is not bounded by $\|\phi\|$. The problem cannot be discarded as mathematical exotics [6]. *Third*, postulating an NHH can lead to inconsistencies for thermal or quantum effects. Even when a microscopic derivation [7, 8] does exist, approximations are usually involved. When those consist of perturbation around a Hermitian theory, one is limited to weak damping. *Fourth*, if $\langle \boldsymbol{f}^j | \boldsymbol{f}_j \rangle = 0$ for some j, then (1.3) fails. This will be our main concern. In this case, $\langle \boldsymbol{f}^j | \boldsymbol{f}_k \rangle = 0$ for *all* k while $\boldsymbol{f}^j \neq 0$, implying that $\{\boldsymbol{f}_k\}$ cannot span the whole space, so that there is a relation to the completeness issue. Obviously the problem does not occur in the Hermitian case $\boldsymbol{f}^j = \boldsymbol{f}_j$, which also means that one cannot convincingly study it in a weak-damping approximation.

In view of the above it is particularly gratifying that, at least in one case, the first three mentioned intricacies are firmly under control. Namely, for a class of one-dimensional open systems, dissipation occurs by leakage of scalar waves from a finite 'cavity' to an infinite 'outside'; the eigenfunctions are the resonances or *quasinormal modes* (QNMs), obeying the outgoing-wave condition (OWC) at the boundary between the two. Starting from the conservative 'universe' of cavity plus outside, one now eliminates the latter *exactly* to arrive at an NHH description for the former alone [9]; this is the analogue of, e.g., integrating out bath variables to derive an effective action [10]. The cavity Green function is fully determined by its QNM poles in the frequency plane [11]. For simple poles this leads to complete BB expansions (1.2) and (1.4) [12]. This has also been verified numerically even for substantial damping[2]. Due to the firm microscopic footing, both canonical [13] and path-integral [14] quantization are possible, in their turn enabling the system to be studied at finite temperatures. For a review, see [15].

[2] For a simple model, in [13] it is shown explicitly that even the infinite-damping limit of the QNM expansion is well behaved.

Provided that non-trivial examples can be found, these systems thus are uniquely suited to study also the fourth intricacy—the normalization problem $\langle \boldsymbol{f}^j | \boldsymbol{f}_j \rangle = 0$—especially given the already stipulated connection to the completeness issue. In fact, one can anticipate that this connection has to do with the *merging of modes*: suppose $\boldsymbol{f}_k \to \boldsymbol{f}_j$ for two (in general $M \geqslant 2$) modes j and k. In the limit, on the one hand one eigenvector is 'lost', so H will no longer be diagonalizable and can be decomposed only into $(M \times M)$ Jordan blocks instead [16]. On the other hand, $\langle \boldsymbol{f}^j | \boldsymbol{f}_j \rangle \to \langle \boldsymbol{f}^j | \boldsymbol{f}_k \rangle = 0$ in the same limit of higher-order modes[3]; this also means that the phenomenon does not occur in conservative, Hermitian systems and indeed is quite different from mere level crossing in the latter[4]. The merging of modes can have spectacular experimental consequences, exemplified by the diverging laser quantum noise reported in [17]. Here, however, we shall be content to have this as a motivation, and focus on the mathematical problem. For QNMs, this should take the form of investigating the higher-order poles which then occur in the Green function.

Therefore, in section 2 we recapitulate the NHH treatment both of the wave equation and of the closely related Klein–Gordon equation. The QNM expansion is derived, assuming that the normalization problem does not occur; the associated duality map arises naturally from the dynamics. Section 3 gives examples of higher-order modes, corresponding to critical damping. Section 4 investigates the resulting block structure of H and introduces basis vectors, replacing the 'lost' eigenvectors, in terms of which this structure assumes a simple normal form. The frequency Green function is still determined by its discrete poles; in section 5 this leads to a complete BB expansion (1.2), (1.3) *even* for higher-order modes, this paper's key result. The BB is generalized in that it does not only involve eigenvectors, but also the 'extra' vectors spanning the Jordan normal form; hence, the dynamics differs from (1.4). Of course, the situation can also be handled by considering merging simple modes, but the limit is singular and requires care. In section 6 we follow the reverse route, developing the perturbation theory which describes how a higher-order mode is split into simple ones [18]. This completes the *exact* BB analysis of our open wave systems by also resolving the fourth delicacy mentioned above. Section 7 contains some concluding remarks.

2. Waves in open systems

2.1. Wave equation

We consider waves in one dimension described by [9, 11, 12, 15]

$$[\rho(x)\partial_t^2 - \partial_x^2]\phi(x,t) = 0 \tag{2.1}$$

on the half line $[0, \infty)$, with $\phi(x{=}0, t) = 0$ and $\phi(x{\to}\infty, t) \to 0$. Let the system S be $[0, a]$ and the bath B be (a, ∞), with $\rho(x > a) = 1$. S and B exchange energy only through $x = a$. The OWC $\partial_t\phi(x,t) = -\partial_x\phi(x,t)$ is imposed in B. The model is relevant for strings [19], electromagnetism [20], and gravity [21]. One must take $\rho > 0$, both physically (ρ is a density [19, 21] or a dielectric constant [20]) and mathematically ((2.2) is singular if $\rho(x_0) = 0$ for some x_0). Hence, ρ can contain a (positive) δ-function, but not δ' or higher (for which (2.2) would be undefined anyway). Thus, ϕ has to be continuous, but ϕ' need not be.

The eigenfunctions or QNMs are factorized solutions $\phi(x,t) = f_j(x)\mathrm{e}^{-\mathrm{i}\omega_j t}$, with

$$[\partial_x^2 + \rho(x)\omega_j^2]f_j(x) = 0 \tag{2.2}$$

[3] If one instead bi-orthonormalizes $\{\boldsymbol{f}_j, \boldsymbol{f}^j\} \mapsto \{\bar{\boldsymbol{f}}_j = \alpha_j \boldsymbol{f}_j, \bar{\boldsymbol{f}}^j = \alpha_j \boldsymbol{f}^j\}$ so that $\langle \bar{\boldsymbol{f}}^j | \bar{\boldsymbol{f}}_j \rangle = 1$, the rescaling thus is singular near the merging point. The normalization problem then manifests itself in that any other measure of the 'size' of $\bar{\boldsymbol{f}}_j$ such as $\langle \bar{\boldsymbol{f}}_j | \bar{\boldsymbol{f}}_j \rangle$ diverges there.

[4] Thus, we shall avoid the terminology 'degeneracy' in this context.

and $f_j(x{>}a) \propto \mathrm{e}^{\mathrm{i}\omega_j x}$. In terms of the momentum $\hat{\phi} = \rho(x)\partial_t\phi$ and the vector

$$\phi = \begin{pmatrix} \phi \\ \hat{\phi} \end{pmatrix}, \tag{2.3}$$

equation (2.1) assumes the Schrödinger form $\mathrm{i}\partial_t\phi = H\phi$ [22], with

$$H = \mathrm{i}\begin{pmatrix} 0 & \rho(x)^{-1} \\ \partial_x^2 & 0 \end{pmatrix}. \tag{2.4}$$

In this two-component form, the eigenvectors are

$$\boldsymbol{f}_j \equiv \begin{pmatrix} f_j \\ \hat{f}_j \end{pmatrix} = \begin{pmatrix} f_j \\ -\mathrm{i}\omega_j\rho f_j \end{pmatrix}. \tag{2.5}$$

The Hamiltonian (2.4) is non-Hermitian, as will be obvious once the appropriate inner product (2.16) is defined. Nevertheless, on the 'universe' $[0, \Lambda]$ (with a node at $x = \Lambda \to \infty$) a complete real spectrum of 'universe modes' is guaranteed to exist. These are given by (2.5) for $\pm\omega_j$, where f_j are the eigenfunctions with eigenvalue ω_j^2 of $-\rho(x)^{-1}\partial_x^2$, which is Hermitian and positive on the 'one-component' space with the product $\langle u, v\rangle = \int_0^\Lambda \mathrm{d}x\, \rho(x)u^*(x)v(x)$. This indirect construction fails on $S = [0, a]$, however. Indeed, the OWC $\hat{\phi}(a^+) = -\phi'(a^+)$ requires two components, and the QNM frequencies have $\mathrm{Im}\,\omega_j < 0$.

2.2. *Green function and poles*

The dynamics is best discussed in terms of the (retarded) Green function, namely

$$\phi(x, t) = \int_0^\infty [G(x, y; t)\hat{\phi}(y) + \partial_t G(x, y; t)\rho(y)\phi(y)]\,\mathrm{d}y \tag{2.6}$$

where ϕ and $\hat{\phi}$ are the initial values of the field and its conjugate momentum. The behaviour of G is determined by the complex singularities of $\tilde{G}(x, y; \omega)$. If (a) $\rho(x)$ has a discontinuity at $x = a$ demarcating S from its surroundings, and (b) $\rho(x{>}a) = 1$ so that outgoing waves are not scattered back into S, the only contributions will be from the isolated QNM poles [11]. If furthermore *all poles are simple*, then in S one can represent G as

$$G(x, y; t) = \mathrm{i}\sum_j \frac{f_j(x)f_j(y)}{(\boldsymbol{f}_j, \boldsymbol{f}_j)}\mathrm{e}^{-\mathrm{i}\omega_j t}. \tag{2.7}$$

Note that the numerator goes as $f_j(x)f_j(y)$, not as e.g. $f_j(x)f_j^*(y)$ (which indeed would violate the symmetry of G in x and y). Thus, the normalization $(\boldsymbol{f}_j, \boldsymbol{f}_j)$, which will turn out to be the same as $\langle \boldsymbol{f}^j | \boldsymbol{f}_j\rangle$ and therefore central to the issue at hand, will have to go as f_j^2, not $|f_j^2|$—a crucial difference, since QNM wavefunctions in general are not real.

Let us derive (2.7) and hence $(\boldsymbol{f}_j, \boldsymbol{f}_j)$ as preparation for section 5. The defining equation

$$D(\omega)\tilde{G}(x, y; \omega) \equiv [\partial_x^2 + \rho(x)\omega^2]\tilde{G}(x, y; \omega) = -\delta(x - y) \tag{2.8}$$

for $0 \leqslant x \leqslant y \leqslant a$ is solved by

$$\tilde{G}(x, y; \omega) = \frac{f(x, \omega)g(y, \omega)}{W(\omega)} \tag{2.9}$$

where f and g obey $D(\omega)f = D(\omega)g = 0$, with $f(x{=}0, \omega) = 0$ and $g(x{>}a, \omega) \propto \mathrm{e}^{\mathrm{i}\omega x}$. The Wronskian $W(\omega) = f'g - fg'$ makes (2.9) independent of the normalization of f and g.

One next closes the Fourier-integral contour for $G(t)$ in the lower half ω-plane. Under the conditions stated, the large semicircle does not contribute and there is no cut caused by

the tail of ρ [11]; one is left with the residues at the zeros[5] ω_j of W. (Without the conditions, there can be non-pole contributions. The QNMs will then be incomplete in a way unrelated to Jordan blocks, leading to short-time transients and long-time power-law tails (say) [23]. Such a 'background' below the resonances will not be discussed here.)

At ω_j, one has $f_j(x) \equiv f(x, \omega_j) = C_j g(x, \omega_j)$. Thus f_j satisfies *both* the left and right boundary conditions, and is a QNM. Assuming for the moment that ω_j is a simple zero, the residue is related to $W'(\omega_j)$, and it is straightforward to show that

$$-C_j \frac{\mathrm{d}W(\omega_j)}{\mathrm{d}\omega} = 2\omega_j \int_0^{a^+} \rho(x) f_j(x)^2 \,\mathrm{d}x + \mathrm{i} f_j(a)^2 \equiv (\boldsymbol{f}_j, \boldsymbol{f}_j). \tag{2.10}$$

The expansion (2.7) for G then follows trivially. In particular, the calculation shows why $(\boldsymbol{f}_j, \boldsymbol{f}_j) \propto f_j^2$ instead of $|f_j^2|$. The definition (2.10) of $(\boldsymbol{f}_j, \boldsymbol{f}_j)$ is valid for QNMs only, and is a special case of (2.13); it shows that the normalization problem is the same as the possibility of higher-order zeros in W, i.e., of merged modes, as was already apparent in section 1.

2.3. Duality

To introduce the duality map, put (2.7) into (2.6), yielding $\phi(t)$ as in (1.4) with[6]

$$a_j = \frac{\mathrm{i}}{(\boldsymbol{f}_j, \boldsymbol{f}_j)} \left\{ \int_0^{a+} [f_j(y)\hat{\phi}(y) + \hat{f}_j(y)\phi(y)] \,\mathrm{d}y + f_j(a)\phi(a) \right\}. \tag{2.11}$$

The OWC has ensured that initial data on the outside $x > a$ do not propagate in, enabling their elimination. We can write (2.11) compactly as

$$a_j = \frac{(\boldsymbol{f}_j, \phi)}{(\boldsymbol{f}_j, \boldsymbol{f}_j)} \tag{2.12}$$

$$(\psi, \chi) \equiv \mathrm{i}\left[\int_0^{a^+} (\psi\hat{\chi} + \hat{\psi}\chi) \,\mathrm{d}x + \psi(a)\chi(a) \right]. \tag{2.13}$$

The bilinear map (2.13) generalizes (2.10)[7]. It (i) in the integral cross-multiplies the two components, and (ii) has no complex conjugation. These suggest a duality operator $\mathcal{D} = \mathcal{F}$, with $\mathcal{F}$ a flip map that (i) swaps the components and (ii) conjugates [24, page 231]

$$\mathcal{F}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \equiv -\mathrm{i}\begin{pmatrix} \psi_2^* \\ \psi_1^* \end{pmatrix} \tag{2.14}$$

so that $\mathcal{F}^2 = \mathbb{I}$. In terms of $\mathcal{F}$, (2.13) can be related to the standard inner product as

$$(\psi, \chi) = \langle \mathcal{F}\psi | \chi \rangle \tag{2.15}$$

$$\langle \zeta | \chi \rangle \equiv \int_0^{\infty} (\zeta^*\chi + \hat{\zeta}^*\hat{\chi}) \,\mathrm{d}x. \tag{2.16}$$

[5] For open systems, the order of the zero of W coincides with the order of the pole in $\tilde{G}$ not only for generic x, y, but in fact for all $x, y > 0$. Namely, a node $f(x_0, \omega_j) = 0$ or $g(x_0, \omega_j) \propto f(x_0, \omega_j) = 0$ would imply zero energy current at position x_0, incompatible with the dissipative nature of the QNMs. This is also relevant in section 5.

[6] In [12], convergence of the QNM expansion is proved for continuous ϕ'' and $(\hat{\phi}/\rho)'$; for discontinuous ϕ the terms need not even tend to zero. Thus, if ϕ is taken in, e.g., L_2 (all square-integrable vectors), $\{\boldsymbol{f}_j, \boldsymbol{f}^j\}$ is not a BB in the mathematical sense but a *spanning* bi-orthogonal system—one which cannot be enlarged because it already spans the whole space. For non-orthogonal systems, bases and spanning sets must be distinguished even in Hilbert space. Hence, expansions such as (1.2), (1.3) at $t = 0$ and (1.4) for $t \geqslant 0$ in fact are valid only in the subspace of smooth functions; this suffices for our Jordan-block analysis. For further information see [25]. Other subtleties, like the surface term in (2.13) seeming ill-defined for functions known only up to L_2 equivalence, or the spatially divergent $\boldsymbol{f}_j$ having infinite norm under (2.16), are also resolved there to complete satisfaction.

[7] In some of our earlier papers, the bilinear map is called a generalized inner product or norm, and sometimes the notation $\langle \psi | \chi \rangle$ is adopted for it.

Hence, (2.11) is of the form (1.3) for $\boldsymbol{f}^j = \mathcal{F}\boldsymbol{f}_j$. The OWC collapses $\int_a^\infty \mathrm{d}x$ in (2.16) to the surface term of (2.13), proving (2.15). That is, (2.15) only holds when either $\boldsymbol{\chi}$ and $\mathcal{F}\boldsymbol{\zeta}$, or $\mathcal{F}\boldsymbol{\chi}$ and $\boldsymbol{\zeta}$, are both outgoing, and only then will the product (2.16) be used. Thus, $\boldsymbol{\chi}$ and $\boldsymbol{\zeta}$ in general belong to different spaces. Since this is unrelated to higher-order poles, these functional-analytic aspects will be dealt with separately [25]. The maps $\mathcal{D}$ and $\mathcal{F}$ are unequal for higher-order poles; however, (2.14) defines $\mathcal{F}$ in general, cf (5.7).

The property (1.1) is equivalent to the symmetry of H under the bilinear map

$$(\boldsymbol{\psi}, H\boldsymbol{\chi}) = (H\boldsymbol{\psi}, \boldsymbol{\chi}). \tag{2.17}$$

To verify (2.17), integrate by parts; the surface term generated cancels the one in (2.13). By an immediate transcription of the standard proof, one now obtains 'orthogonality'

$$(\boldsymbol{f}_j, \boldsymbol{f}_k) = 0 \qquad j \neq k. \tag{2.18}$$

What remains is to show that higher-order zeros in W can indeed exist (section 3), and to generalize the above formalism to those cases (sections 4–6).

2.4. Klein–Gordon equation

Also of interest in this context is the Klein–Gordon equation describing, *inter alia*, the propagation of linearized gravitational waves on a curved black-hole background [26]

$$[\partial_t^2 - \partial_x^2 + V(x)]\phi(x,t) = 0. \tag{2.19}$$

Essentially the same formalism applies, *mutatis mutandis* [27]. The discontinuity condition (a) now refers to V, and the no-tail condition (b) reads $V(x>a) = 0$. Elsewhere we replace $\rho \mapsto 1$, $-\partial_x^2 \mapsto -\partial_x^2 + V(x)$. An example in terms of (2.19) will be given below.

3. Higher-order poles

3.1. General remarks

For one-dimensional *conservative* systems, e.g. (2.2) with nodes at $x = 0$ and a, W can only have simple zeros since in (2.10) the surface term is now absent, while the integral is positive definite up to an overall phase. Thus, their eigenfrequencies have a finite spacing $\Delta\omega$, and can be labelled by the number of nodes of the corresponding eigenfunctions. Hence, it is by no means obvious that higher-order poles can exist in the case of outgoing waves. Therefore, we will give some examples (cf [28]) before studying the extension of the BB formalism.

Any pole of order $M > 1$, when suitably perturbed, splits into M first-order ones, as shown explicitly in section 6. The coalescence of poles contemplated in section 1 thus is generic, as is the 'loss' of modes: when simple poles merge, there is only *one* eigenfunction left—in contrast to the case of degeneracies in conservative systems. Namely, for a given ω, the conditions $f(x=0,\omega) = 0$ and $f'(x=0,\omega) = 1$, say, uniquely specify f. The $M-1$ 'missing' modes make the possibility of higher-order poles all the more interesting.

For simplicity, here we concentrate on second-order poles. Proving the existence of third-order poles and discussing other possibilities is deferred to appendix A. It is best to look for double poles on the imaginary axis in the ω-plane. First, apart from some overall factors of i, the problem then is purely real and easy to handle. More physically, as the system parameter(s) are tuned, it is 'unlikely' that two poles in the complex plane would collide—not only would this require simultaneously tuning two parameters, but one also expects level repulsion[8]. However,

[8] QNM time-independent perturbation theory is analogous to the conservative case [12]. Generically it leads to level repulsion in one direction in the ω-plane, and attraction in the other. The trajectories of two modes would then be like a pair of hyperbolas which come close without touching; cf the examples for absorptive systems in [11].

QNMs of the dissipative system (2.1) exist in pairs, with frequencies ω and $-\omega^*$ lying on the same horizontal line. It would require the tuning of only *one* parameter to make them collide, which they must do on the imaginary axis. In fact, we expect that after they collide, the two poles will move apart along this axis, in exact analogy to an oscillator going through critical damping. This scenario is exemplified in both models shown below, and it remains an open question whether higher-order poles can exist off the imaginary axis for our class of open systems.

3.2. Example in the wave equation

With these remarks, we look for a double zero of W for the wave equation at $\omega = -\mathrm{i}\gamma$, $\gamma > 0$. The differential equation (suppressing the mode index[9] j) then becomes real

$$[\partial_x^2 - \rho(x)\gamma^2]f(x) = 0 \tag{3.1}$$

and the eigenvalue condition is $f'/f = \gamma$ at $x = a^+$, which ensures that $W(-\mathrm{i}\gamma) = 0$. For ω to be a double zero, we also need $(\boldsymbol{f}, \boldsymbol{f}) \propto W'(-\mathrm{i}\gamma)$ to vanish

$$\mathrm{i}(\boldsymbol{f}, \boldsymbol{f}) = 2\gamma \int_0^{a^+} \rho(x) f(x)^2 \,\mathrm{d}x - f(a)^2 = 0. \tag{3.2}$$

Using (3.1) to express $\rho(x)f(x)$ in terms of f'' and then integrating by parts, this becomes

$$\mathrm{i}(\boldsymbol{f}, \boldsymbol{f}) = -\frac{2}{\gamma} \int_0^a f'^2 \,\mathrm{d}x + f(a)^2 = 0. \tag{3.3}$$

The last term has been reversed by the surface term $-2f(a)^2$ from the integration by parts.

Interestingly, ρ does not appear in (3.3), and this is central to the following construction.

(i) Choose any function f satisfying $f(x{=}0) = 0$, $f'(x{=}0) > 0$, and $f'' > 0$.
(ii) Use (3.3) to determine γ.
(iii) Put these back into (3.1) to find ρ, which is guaranteed to be positive.

There is, however, one further subtlety. Such a construction gives $f'(a^-)$, and also $f'(a^+) = \gamma f(a)$; the difference between the two must be attributed, through (3.1), to $\rho(x) = \cdots + \mu\delta(x-a)$, with $\mu = \gamma^{-1} - f'(a^-)/(\gamma^2 f(a))$. One must check that $\mu \geqslant 0$, i.e., that

$$2\int_0^a f'^2 \,\mathrm{d}x \geqslant f(a)f'(a^-). \tag{3.4}$$

This condition is non-trivial, and for instance violated for some α if $f(x) = x + \alpha x^n$, $n \geqslant 5$.

Yet examples abound, e.g.

$$f(x{<}1) = \sinh(Kx) \tag{3.5a}$$

$$\gamma = K\,\mathrm{cotanh}K + \frac{K^2}{\sinh^2 K} \tag{3.5b}$$

$$\rho(x) = \frac{K^2}{\gamma^2}\theta(1-x) + \frac{K^2}{\gamma^2 \sinh^2 K}\delta(x-1) + \theta(x-1) \tag{3.5c}$$

(so that $a = 1$), for any $K > 0$. Note that always $\rho(0{<}x{<}1) = K^2/\gamma^2 < 1$, the case in which there is a zero-mode even if the δ-term in (3.5*c*) is absent [12, 13]. Incidentally, this case without the δ-term thus already shows that the open string (2.1) can exhibit features not found in damped harmonic oscillators, as will become even clearer in appendix A.

[9] Following our conventions in previous papers [12, 13], QNMs on the negative imaginary ω-axis will be termed zero-modes and labelled with $j = 0$ if necessary.

3.3. Example in the Klein–Gordon equation

We next give an example for the Klein–Gordon equation, which may appear more natural in that the system (i.e., $V(x)$) is specified in advance and not obtained as an answer.

Recall the Pöschl–Teller potential [29]

$$V(x) = \mathcal{V}\,\mathrm{sech}^2 x. \tag{3.6}$$

The model is exactly soluble, with the eigenvalues given by[10]

$$\omega_j^{\pm} = \begin{cases} \pm\sqrt{\mathcal{V} - \frac{1}{4}} - \mathrm{i}(j + \frac{1}{2}) & \text{if} \quad \mathcal{V} \geqslant \frac{1}{4} \\ -\mathrm{i}\left[j + \frac{1}{2} \pm \sqrt{\frac{1}{4} - \mathcal{V}}\right] & \text{if} \quad \mathcal{V} \leqslant \frac{1}{4} \end{cases} \tag{3.7}$$

$j = 0, 1, 2, \ldots$. Each pair of poles merge at $\mathcal{V} = \frac{1}{4}$, where the damping becomes critical.

This example is slightly unsatisfactory in one way: V has no discontinuity but does have a tail (i.e., it does not vanish outside some finite interval), so the QNMs would not be complete even when all poles are first order. We may consider a minor alteration: if $V(|x|>a) \mapsto 0$ for some large a, one would expect the $\omega_j^{\pm}$ to be little changed. Actually this is not true in general [30], but this subtlety is not related to the present issue. Here it suffices that at least the *first* mode pair $j = 0$ are not much affected by truncation, in that the $a \to \infty$ limit recovers their position for the untruncated V. At critical damping these then demonstrate a double zero of W in a context where the QNMs are otherwise complete. We have found this double zero numerically at $a = 5$, $\mathcal{V} = 0.252\,279\,109\ldots$, $\mathrm{i}\omega = 0.511\,109\ldots$.

4. Jordan blocks

With the possibility of Mth-order zeros of W ($M \geqslant 2$) established, in this section we focus on the subspace associated with a single such zero ω_j. As mentioned in section 3.1, in this subspace there is only one eigenvector; presently $M - 1$ other basis vectors will be obtained. Thus, this $M \times M$ block in H is not diagonalizable. From now on, we will only discuss the wave equation (2.1).

Using the definitions below (2.9), the (position-independent) Wronskian can be written as $W(\omega) = f'(0,\omega)g(0,\omega)$. One proves by induction that $\partial_\omega^n g(0,\omega)|_{\omega_j} = 0$ for $0 \leqslant n \leqslant M-1$ ($f'(x{=}0) \neq 0$ since otherwise $f(x) \equiv 0$). Hence, up to this order in $\omega - \omega_j$, the functions f and g satisfy the same boundary conditions and can be normalized to be equal: if we define

$$f(x,\omega) = \sum_{n=0}^{M-1} f_{j,n}(x)(\omega - \omega_j)^n + \mathcal{O}[(\omega - \omega_j)^M] \tag{4.1}$$

so that $f_{j,n}(x) \equiv (1/n!)\partial_\omega^n f(x,\omega)|_{\omega_j}$, then we also have

$$g(x,\omega) = \sum_{n=0}^{M-1} f_{j,n}(x)(\omega - \omega_j)^n + \mathcal{O}[(\omega - \omega_j)^M]. \tag{4.2}$$

Now for $0 \leqslant n \leqslant M-1$ define

$$\begin{aligned} f_{j,n}(x,t) &\equiv \frac{1}{n!}\partial_\omega^n [f(x,\omega)\mathrm{e}^{-\mathrm{i}\omega t}]_{\omega_j} = \frac{1}{n!}\partial_\omega^n [g(x,\omega)\mathrm{e}^{-\mathrm{i}\omega t}]_{\omega_j} \\ &= \sum_{m=0}^{n} f_{j,n-m}(x)\frac{(-\mathrm{i}t)^m}{m!}\mathrm{e}^{-\mathrm{i}\omega_j t} \end{aligned} \tag{4.3}$$

[10] Here the Klein–Gordon equation is considered on the full line $-\infty < x < \infty$ rather than on $0 \leqslant x < \infty$. Only trivial changes are required in the formalism; see, e.g., [11, 23, 27].

where the last line follows using (4.2). These are not only outgoing solutions of the wave equation (since $g(x,\omega)\mathrm{e}^{-\mathrm{i}\omega t}$ is for any ω), but have a node at the origin as well (since $f(x,\omega)\mathrm{e}^{-\mathrm{i}\omega t}$ has one for any ω). The associated momenta are

$$\begin{aligned}\hat{f}_{j,n}(x,t) &\equiv \rho(x)\dot{f}_{j,n}(x,t)\\ &= -\mathrm{i}\rho(x)[\omega_j f_{j,n}(x,t) + f_{j,n-1}(x,t)]\end{aligned} \tag{4.4}$$

so that the action of the Hamiltonian is $H\boldsymbol{f}_{j,n} = \omega_j \boldsymbol{f}_{j,n} + \boldsymbol{f}_{j,n-1}$, with $\boldsymbol{f}_{j,-1} \equiv 0$.

For fixed j, the functions $\{f_{j,n}(x,t)\}_{n=0}^{M-1}$ are linearly independent (in that a non-trivial superposition cannot vanish identically in x and t), as is obvious by looking at the highest power of t in each (the coefficient of $t^n\mathrm{e}^{-\mathrm{i}\omega_j t}$ in $f_{j,n}$ is $\propto f_j(x)$, which by definition is non-zero). Therefore the initial data $\boldsymbol{f}_{j,n}$ have to be independent as well[11], otherwise one would have a vanishing superposition evolving into a non-vanishing function.

Thus the set $\{\boldsymbol{f}_{j,n}\}_{n=0}^{M-1}$ is a basis, in which the Hamiltonian reads

$$H = \begin{pmatrix} \omega_j & 1 & 0 & \cdots & 0 \\ 0 & \omega_j & 1 & \cdots & 0 \\ 0 & 0 & \omega_j & \ddots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \omega_j \end{pmatrix}. \tag{4.5}$$

While it is guaranteed that H can be cast into the so-called *Jordan normal form* (4.5) in a subspace with precisely one eigenvector [16], we have now established a basis with respect to which this is indeed the case, and related this basis to the solutions $f(x,\omega)$, $g(x,\omega)$. The basis is not unique, since rescaling $f(x,\omega) \mapsto \mathcal{N}(\omega)f(x,\omega)$ mixes the $f_{j,n}$, with only $f_j = f_{j,0}$ remaining invariant up to a prefactor; in fact, this rescaling is readily checked to generate precisely those basis transformations which leave the form (4.5) for H invariant. A further—essentially unique—specification of the basis will be made in section 5.

Vectors from different blocks are 'orthogonal' under the bilinear map (2.13), i.e.

$$(\boldsymbol{f}_{j,n}, \boldsymbol{f}_{k,m}) = 0 \qquad j \neq k. \tag{4.6}$$

The proof proceeds by induction with respect to $n+m$. The case $n+m=0$ is the standard one of eigenvectors given in (2.18). Now consider

$$\begin{aligned}\omega_j(\boldsymbol{f}_{j,n}, \boldsymbol{f}_{k,m}) + (\boldsymbol{f}_{j,n-1}, \boldsymbol{f}_{k,m}) &= (H\boldsymbol{f}_{j,n}, \boldsymbol{f}_{k,m}) = (\boldsymbol{f}_{j,n}, H\boldsymbol{f}_{k,m})\\ &= \omega_k(\boldsymbol{f}_{j,n}, \boldsymbol{f}_{k,m}) + (\boldsymbol{f}_{j,n}, \boldsymbol{f}_{k,m-1}).\end{aligned} \tag{4.7}$$

On both sides, the second terms vanish by the induction hypothesis, so one is left with $(\omega_j - \omega_k)(\boldsymbol{f}_{j,n}, \boldsymbol{f}_{k,m}) = 0$, proving (4.6).

5. Generalized bi-orthogonal expansion

Having obtained the extra non-eigenvector solutions $f_{j,n\geqslant 1}(x,t)$, we now investigate their role in the field expansion. We shall consider all poles simultaneously, so that the block size M acquires an index j. As with the Jordan normal form of H (cf below (4.5)), a basis dual to

[11] The $\boldsymbol{f}_{j,n}$ being linearly independent of course does not mean that they are unrelated. In fact, taking $\partial_\omega[D(\omega)f(x,\omega) = 0]$ and solving the ensuing $D(\omega_j)f_{j,1} = -2\omega_j\rho f_j$ by variation of the constant, one finds (for $M \geqslant 2$) $f_{j,1}(x) = 2\omega_j f_j(x)\int_x \mathrm{d}y\, f_j^{-2}(y)\int_0^y \mathrm{d}z\, \rho(z) f_j^2(z)$, where the undetermined constant of integration corresponds to the freedom pointed out below (4.5). For $M \geqslant 3$, higher derivatives can be calculated similarly. However, the expressions in the main text are more transparent if the $f_{j,n}$ are left unevaluated.

$\{\boldsymbol{f}_{j,n}\}_{n=0}^{M_j-1}$ is known to exist on general grounds (see appendix B), but it remains to find its explicit form and, if possible, to choose the original basis (still subject to the freedom pointed out below (4.5)) so that the ensuing expressions are as simple as possible.

Our starting point is (2.6), with $G(x, y; t) = \int(\mathrm{d}\omega/2\pi)\tilde{G}(x, y; \omega)\mathrm{e}^{-\mathrm{i}\omega t}$ and $\tilde{G}$ given by (2.9). Consider an M_jth-order zero[5] of the Wronskian,

$$\begin{aligned} W(\omega) &= W_{j,M_j}(\omega-\omega_j)^{M_j}\mathcal{M}(\omega) \\ &= W_{j,M_j}(\omega-\omega_j)^{M_j} + \mathcal{O}[(\omega-\omega_j)^{M_j+1}] \end{aligned} \tag{5.1}$$

with $\mathcal{M}(\omega_j) = 1$. We now use the remaining freedom $f \mapsto \mathcal{N}f$, taking $\mathcal{N}(\omega) = \mathcal{M}(\omega)^{-1/2} + \mathcal{O}[(\omega-\omega_j)^{M_j}]$ (analytic near $\omega = \omega_j$) and similarly for g, preserving (4.2). One obtains[12]

$$W(\omega) = W_{j,M_j}(\omega-\omega_j)^{M_j} + \mathcal{O}[(\omega-\omega_j)^{2M_j}] \tag{5.2}$$

where we draw attention to the order of the error term. Equation (5.2) will greatly simplify the formulae below. The contour integral for G is now straightforward, leading to

$$G(x, y; t) = \sum_j \frac{\mathrm{e}^{-\mathrm{i}\omega_j t}}{\mathrm{i}W_{j,M_j}} \sum_{n=0}^{M_j-1}\sum_{m=0}^{n} f_{j,m}(y) f_{j,n-m}(x) \frac{(-\mathrm{i}t)^{M_j-1-n}}{(M_j-1-n)!} \tag{5.3}$$

($t \geqslant 0$ throughout this section). By symmetry, (5.3) also holds for $0 \leqslant y < x \leqslant a$ even though this is not the case for the original (2.9). If $M_j = 1$ for all j, this agrees with the combination of (2.7) and (2.10). In general, one can rewrite

$$G(x, y; t) = \sum_j \frac{1}{\mathrm{i}W_{j,M_j}} \sum_{n=0}^{M_j-1} f_{j,M_j-1-n}(y) f_{j,n}(x, t) \tag{5.4}$$

with $f_{j,n}(x, t)$ defined in (4.3). Insertion into (2.6) yields the time evolution

$$\phi(x, t) = -\sum_j \frac{1}{W_{j,M_j}} \sum_{n=0}^{M_j-1} (\boldsymbol{f}_{j,M_j-1-n}, \phi) f_{j,n}(x, t) \tag{5.5}$$

in terms of the bilinear map (2.13). In particular, this holds for $\phi = \boldsymbol{f}_{k,m}$. Then, terms with $j \neq k$ vanish by (4.6), and the linear independence of the $f_{k,n}(t)$ discussed above (4.5) implies that the coefficients on both sides of (5.5) are equal, i.e.

$$(\boldsymbol{f}_{j,n}, \boldsymbol{f}_{k,m}) = -W_{j,M_j}\delta_{jk}\delta_{n+m,M_j-1}. \tag{5.6}$$

Of course, this intra-block 'orthogonality' is conditional on the normalization $W^{(n)}(\omega_j) = 0$ for $M_j + 1 \leqslant n \leqslant 2M_j - 1$, imposed in (5.2); otherwise one has (5.13) below instead. In view of (2.15), the relation (5.6) leads one to define

$$\boldsymbol{f}^{j,n} \equiv \mathcal{D}\boldsymbol{f}_{j,n} \equiv \mathcal{F}\boldsymbol{f}_{j,M_j-1-n} \tag{5.7}$$

where $\mathcal{F}$ is the flip operation in (2.14). Thus

$$\langle \boldsymbol{f}^{j,n} | \boldsymbol{f}_{j',n'} \rangle = -W_{j,M_j}\delta_{jj'}\delta_{nn'} \tag{5.8}$$

where $W_{j,M_j} \neq 0$ by definition, cf (5.1), solving the normalization problem. The result (5.8) is significant; it shows that, unless $M_j = 1$ for all j, the duality map $\mathcal{D}$ no longer coincides with $\mathcal{F}$ in that $\mathcal{D}$ changes the intra-block index n of $\boldsymbol{f}_{j,n}$. Since the flip map obeys

$$\mathcal{F}H = H^\dagger\mathcal{F} \tag{5.9}$$

[12] One has $W_{j,M_j+n} = \sum_{m=0}^{n} f'_{j,n-m}(0)g_{j,M_j+m}(0)$, and for $n \leqslant M_j - 1$ this does *not* depend on the choice of g_{j,M_j+m}. Namely, $g(x, \omega) \mapsto [1 + (\omega-\omega_j)^{M_j}\mathcal{N}(\omega)]g(x, \omega)$ yields $g_{j,M_j+m} \mapsto g_{j,M_j+m} + \sum_{\ell=0}^{m}\mathcal{N}_{j,m-\ell}g_{j,\ell}$, with $g_{j,\ell}(0) = 0$ since $\ell \leqslant M_j - 1$. Thus (5.2) only depends on the normalization of f and g up to order M_j, as stated in the main text. Cf (5.13) where, at the expense of a slightly more involved calculation, $W_{j,n\leqslant 2M_j-1}$ is expressed in a form which *manifestly* involves only $f_{j,m}$, $g_{j,m}$ for $m \leqslant M_j - 1$.

(the proof outlined below (2.17) does not invoke any assumptions on the block structure of H) the relation (1.1) in general is *not* satisfied by the operator $\mathcal{D}$ implicit in (1.3). Since it is an immediate consequence of (5.9) that $\mathcal{F}$ carries right into left eigenvectors and vice versa, the left eigenvector corresponding to $\boldsymbol{f}_j = \boldsymbol{f}_{j,0}$ is $\mathcal{F}\boldsymbol{f}_{j,0} = \boldsymbol{f}^{j,M_j-1} \neq \boldsymbol{f}^{j,0}$ for $M_j > 1$. While the left and right eigenvectors thus are orthogonal as stipulated in section 1, this does not lead to normalization problems as these vectors are not each other's dual.

Using (5.6) and (5.7), the final results for the generalized BB expansion become

$$G(x, y; t) = \mathrm{i} \sum_j \sum_{n=0}^{M_j-1} \frac{f_{j,M_j-1-n}(y) f_{j,n}(x, t)}{(\boldsymbol{f}_{j,M_j-1-n}, \boldsymbol{f}_{j,n})} \tag{5.10}$$

$$\phi(t) = \sum_j \sum_{n=0}^{M_j-1} \frac{\langle \boldsymbol{f}^{j,n} | \phi \rangle}{\langle \boldsymbol{f}^{j,n} | \boldsymbol{f}_{j,n} \rangle} \boldsymbol{f}_{j,n}(t). \tag{5.11}$$

The $t \downarrow 0$ limit of $G(x, y; t)$ then yields the sum rule

$$\mathrm{i} \sum_j \sum_{n=0}^{M_j-1} \frac{f_{j,M_j-1-n}(y)}{(\boldsymbol{f}_{j,M_j-1-n}, \boldsymbol{f}_{j,n})} \begin{pmatrix} f_{j,n}(x) \\ \hat{f}_{j,n}(x) \end{pmatrix} = \begin{pmatrix} 0 \\ \delta(x - y) \end{pmatrix} \tag{5.12}$$

while in the same limit, (5.11) is indeed seen to be of the form (1.2), (1.3).

Equation (5.6) is the generalization of (2.10) and (2.18), while our proof is a slight simplification even for simple poles [11]. The representation (5.10) generalizes (2.7), and (5.11) extends (1.4) and (2.12). Also the simple-pole case of (5.12) is already known [11].

One may ask to what extent the basis we have obtained is unique. On the one hand we demand that the Hamiltonian have the normal form (4.5), and below this equation it has already been remarked that this forces the functions $f_{j,n}$ to be of the form (4.3) for some normalization of $g(x, \omega)$. On the other hand, to ensure the simplicity of formulae like (5.11), we require that the dual to $\boldsymbol{f}_{j,n}$ be some $\mathcal{F}\boldsymbol{f}_{j',n'}$, where (4.6) then forces $j' = j$. Now for *any* normalization of f and g (i.e., temporarily abandoning (4.2) and (5.2)) one has

$$(\boldsymbol{f}_{j,n}, \boldsymbol{g}_{j,m}) = -W_{j,n+m+1} \tag{5.13}$$

as long as $n, m \leqslant M_j - 1$ (implying that the bilinear map vanishes if $n + m \leqslant M_j - 2$), as can be proved by operating with $\sum_{\ell=0}^{n} [(n-\ell)!(m+\ell+1)!]^{-1} \partial_\omega^{n-\ell} \partial_{\omega'}^{m+\ell+1}|_{\omega=\omega'=\omega_j}$ on the identity

$$(\omega^2 - \omega'^2) \int_0^{a^+} \rho f(\omega) g(\omega') \, \mathrm{d}x = [\mathrm{i}\omega' f(a, \omega) - f'(a^+, \omega)] g(a, \omega') + f'(0, \omega) g(0, \omega'). \tag{5.14}$$

Hence, always $(\boldsymbol{f}_{j,n}, \boldsymbol{f}_{j,M_j-1-n}) \neq 0$, and the only way to bi-orthogonalize by setting other products to zero as in (5.6) is normalizing W as in (5.2), obviously fixing the $\boldsymbol{f}_{j,n}$ up to one overall prefactor per Jordan block. Thus, our basis is unique up to these prefactors. In fact, further analogy to the customary treatment [15] of simple poles results if $f(x, \omega)$ is chosen such that $W_{j,M_j} = -2\omega_j$ for all j, implying $(\boldsymbol{f}_{j,n}, \boldsymbol{f}_{k,m}) = 2\omega_j \delta_{jk} \delta_{n+m,M_j-1}$. This preferential normalization (convenient in applications [14]) reduces the freedom to one sign per block.

In closing, let us return to the example of section 3.2 with $M = 2$. Using either (4.1) or the integral representation[11], one finds the 'preferred' second basis function (i.e., the one for which[9] $(\boldsymbol{f}_{0,1}, \boldsymbol{f}_{0,1}) = 0$) corresponding to $f_0 = f$ as in (3.5*a*) to be

$$f_{0,1}(x) = f_a(x) + f_b(x) \tag{5.15a}$$

$$f_a(x) = \mathrm{i} \frac{K}{\gamma} x \cosh(Kx) \tag{5.15b}$$

$$f_b(x) = -\mathrm{i} \left(\frac{2}{3} \frac{K}{\gamma} + \frac{1}{2K} \right) \tanh K \sinh(Kx). \tag{5.15c}$$

The conjugate momentum $\hat{f}_{0,1}$ is given by (4.4). While (5.15) is given here for reference and further use in section 6, there does not seem to be a simple physical interpretation. The normalization occurring in the field expansion (5.11) is evaluated as

$$\langle \boldsymbol{f}^0 | \boldsymbol{f}_0 \rangle = \langle \boldsymbol{f}^{0,1} | \boldsymbol{f}_{0,1} \rangle = (\boldsymbol{f}_0, \boldsymbol{f}_{0,1}) = \frac{K^3}{\gamma^2} \mathrm{cotanh} K. \tag{5.16}$$

Since the contribution of f_b to the product (5.16) is proportional to $(\boldsymbol{f}_0, \boldsymbol{f}_0)$, it vanishes. However, in a calculation in section 6.3 this term in $f_{0,1}$ will be essential for arriving at the correct result.

6. Jordan-block perturbation theory

6.1. Formalism for the generic case

The use of BBs places dissipative systems into a framework very similar to that for conservative ones, so that time-independent perturbation theory can be transcribed from textbook results. Nevertheless, these now apply to *complex* eigenvalues and shifts [12][13].

Let us investigate how this formalism, previously developed for simple QNM spectra, is modified if at least one ω_j is associated with a non-trivial Jordan block. The ensuing splitting of the multiple pole into M_j distinct ones (in the generic case, defined below) is reminiscent of the lifting of a degeneracy by a perturbation (typically breaking some symmetry) in Hermitian systems; however, important differences exist. First, of the M_j degrees of freedom in the block, only one is an eigenvector, as emphasized before. Second, for Jordan blocks the splitting generically is governed by only *one* complex parameter α; hence, the M_j frequency shifts are not independent. In fact, all their relative magnitudes and phases are predetermined, and only the overall values depend on the details of the perturbation through α; cf (6.4). While this may seem unusual, it actually simplifies the calculation.

While Jordan-block perturbations thus differ essentially from those of degenerate levels in closed systems, we will study the former by a method also used for the latter: transferring part of the perturbing NHH H' to the unperturbed H_0 and treating this part exactly, upon which the remainder of H' can be dealt with using non-degenerate perturbation theory.

Specifically, let $H = H_0 + \lambda H'$, where H_0 is assumed to have a known Jordan normal form as described in sections 4 and 5, H' accounts for a change in density $\delta(\rho^{-1})$, and where $|\lambda| \ll 1$. For simplicity, it is supposed that there is only one $M_j \geqslant 2$; the generalization to several Jordan blocks is immediate. Consider the splitting part of H'

$$H'_{\mathrm{s}} \phi \equiv \frac{\boldsymbol{f}_{j,M_j-1} \langle \boldsymbol{f}^{j,M_j-1} | H' \boldsymbol{f}_j \rangle \langle \boldsymbol{f}^j | \phi \rangle}{\langle \boldsymbol{f}^{j,M_j-1} | \boldsymbol{f}_{j,M_j-1} \rangle \langle \boldsymbol{f}^j | \boldsymbol{f}_j \rangle}. \tag{6.1}$$

This has only one non-vanishing matrix element, namely

$$\alpha \equiv \frac{\langle \boldsymbol{f}^{j,M_j-1} | H' \boldsymbol{f}_j \rangle}{\langle \boldsymbol{f}^{j,M_j-1} | \boldsymbol{f}_{j,M_j-1} \rangle} = \frac{(\boldsymbol{f}_j, H' \boldsymbol{f}_j)}{(\boldsymbol{f}_{j,M_j-1}, \boldsymbol{f}_j)} \tag{6.2}$$

$$= \frac{\omega_j^2 \int_0^{a^+} \delta(\rho^{-1}) \rho^2 f_j^2 \, \mathrm{d}x}{(\boldsymbol{f}_{j,M_j-1}, \boldsymbol{f}_j)}. \tag{6.3}$$

We transfer this part to the unperturbed Hamiltonian: $\tilde{H}_0 \equiv H_0 + \lambda H'_{\mathrm{s}}$, so that the remainder is $\tilde{H}' = H' - H'_{\mathrm{s}}$. The perturbation is said to be generic iff $\alpha \neq 0$. This definition will be

[13] In [12], the duality transformation is not explicitly mentioned. Rather, bilinear maps (ψ, χ) are used; these can be cast into the BB language by (2.15).

justified below, by showing that $\tilde{H}'$ effects only a higher-order correction in λ compared to the splitting caused by $\alpha \neq 0$. First of all, however, note that for an infinitesimal $\delta\rho$, (6.3) implies $\alpha \propto \int_0^{a^+} \delta\rho f_j^2 \,\mathrm{d}x$. Using this and the variation-of-constant method (cf the inner integrand in footnote 11), $\alpha \neq 0$ is seen to be equivalent to $\partial_\lambda g(0,\omega_j) \propto \partial_\lambda W(\omega_j) \neq 0$. In other words, if $\alpha \neq 0$ the M_jth-order zero in the Wronskian is split already in the lowest order.

In the $M_j \times M_j$ block associated with ω_j, one finds $\det(\tilde{H}_0 - \omega\mathbb{1}) = (\omega_j - \omega)^{M_j} - (-)^{M_j}\lambda\alpha$ for the characteristic polynomial. This yields the eigenfrequencies of $\tilde{H}_0$ as

$$\tilde{\omega}_j^{(n)} = \omega_j + s\mathrm{e}^{2\pi n\mathrm{i}/M_j} \tag{6.4}$$

($0 \leqslant n \leqslant M_j - 1$), where $s = \sqrt[M_j]{\lambda\alpha}$ is an arbitrary but fixed choice of the root. Thus, the splittings $\tilde{\omega}_j^{(n)} - \omega_j$ all have the same magnitude $\propto \lambda^{1/M_j}$ and are equiangular. Both their magnitude and the overall phase are determined by α. The eigenvectors of $\tilde{H}_0$ are

$$\tilde{\boldsymbol{f}}_j^{(n)} = \sum_{m=0}^{M_j-1} s^m \mathrm{e}^{2\pi nm\mathrm{i}/M_j} \boldsymbol{f}_{j,m}. \tag{6.5}$$

Since the higher-order pole has been split into first-order ones, their duals read simply

$$\tilde{\boldsymbol{f}}_{(n)}^{j} = \mathcal{F}\tilde{\boldsymbol{f}}_j^{(n)}. \tag{6.6}$$

It remains to account for $\tilde{H}'$, using conventional perturbation theory, by evaluating its matrix in the new basis. The validity of this procedure is not entirely trivial, since the transformation from $\{\boldsymbol{f}_{j,m}\}$ to $\{\tilde{\boldsymbol{f}}_j^{(n)}\}$, effected by $P_{mn} = s^m \mathrm{e}^{2\pi nm\mathrm{i}/M_j}$, becomes singular if $\lambda \to 0$. For a justification, denote the old matrix elements as $\tilde{H}'_{nm} = \langle \boldsymbol{f}^{j,n}|\tilde{H}'\boldsymbol{f}_{j,m}\rangle / \langle \boldsymbol{f}^{j,n}|\boldsymbol{f}_{j,n}\rangle$, and evaluate the inverse transform (in fact a discrete Fourier inversion) as $(P^{-1})_{mn} = M_j^{-1} s^{-n} \mathrm{e}^{-2\pi nm\mathrm{i}/M_j}$. In the basis diagonalizing $\tilde{H}_0$, the perturbation then reads

$$\begin{aligned} \frac{\langle \tilde{\boldsymbol{f}}_{(n)}^{j}|\tilde{H}'\tilde{\boldsymbol{f}}_j^{(m)}\rangle}{\langle \tilde{\boldsymbol{f}}_{(n)}^{j}|\tilde{\boldsymbol{f}}_j^{(n)}\rangle} &= \sum_{k,\ell=0}^{M_j-1} (P^{-1})_{nk} \tilde{H}'_{k\ell} P_{\ell m} \\ &= \sum_{k,\ell=0}^{M_j-1} \frac{1}{M_j} \mathrm{e}^{2\pi(\ell m - nk)\mathrm{i}/M_j} \tilde{H}'_{k\ell} s^{\ell-k}. \end{aligned} \tag{6.7}$$

Crucially, the power s^{1-M_j} does not occur since $\tilde{H}'_{M_j-1,0} = 0$ on account of (6.1). Thus the matrix elements of $\lambda\tilde{H}'$ are $\mathcal{O}(s^{M_j}s^{2-M_j})$, which means that the first-order frequency shifts due to $\tilde{H}'$ are $\mathcal{O}(s^2)$, small compared to the lowest-order splittings $\Delta\tilde{\omega}_j^{(n)} \propto s$. With 'energy' denominators $\tilde{\omega}_j^{(n)} - \tilde{\omega}_j^{(m)} \propto s$, higher-order shifts are smaller still by successive powers[14] of s. Of course, inter-block matrix elements of $\tilde{H}'$ can be handled without difficulty.

6.2. Nongeneric case

If $\alpha = 0$ the leading behaviour is determined by other matrix elements, and the splitting of ω_j can be partial or, depending on the scheme of calculation, occurs only in higher order [18]. We

[14] In fact, this last statement on the smallness of higher-order corrections is the more relevant one. Namely, the textbook formula for the lowest-order *wavefunction* correction already has an energy denominator, unlike for the frequency shift. Hence, the contribution of $\tilde{H}'$ is $\mathcal{O}(s)$, so that the lowest order is *not* given by (6.5) alone, in contrast to (6.4). (However, the part of the $\mathcal{O}(s)$-correction not due to H'_{s} is $\propto \boldsymbol{f}_j$, and thus can be absorbed into a change of normalization.) Still, after the transformation (6.5), one obtains a well-defined perturbation expansion also for the QNM wavefunctions.

shall not investigate the general case, but instead give an example relevant to the discussion in appendix A. Namely, if a 4×4 Jordan block is perturbed by

$$H' = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \alpha & 0 \end{pmatrix} \tag{6.8}$$

(in the normal-form basis $\{\boldsymbol{f}_{j,n}\}$), one finds $\det(H - \omega \mathbb{1}) = [(\omega - \omega_j)^2 - \lambda\alpha]^2$. Thus, the fourth-order pole is split into two second-order ones, and the latter do not undergo further splitting to any order. Of course, this treatment does not address the question whether for some $\delta\rho$ the perturbation H' can have the form (6.8) for the open system (2.1), even if a fourth-order pole is assumed to exist. However, H' as in (6.8) at least satisfies the fundamental $\langle \boldsymbol{f}^{j,n} | H' \boldsymbol{f}_{j,m} \rangle = \langle \boldsymbol{f}^{j,M_j-1-m} | H' \boldsymbol{f}_{j,M_j-1-n} \rangle$ (i.e., reflection symmetry with respect to the NE–SW diagonal within one block), which follows from (2.17) and (5.7).

6.3. Example

Returning to the example (3.5) of section 3.2, and bearing in mind the NHH action (2.4) on a two-component vector[15], we study the perturbation $\rho^{-1}(x) \mapsto \rho^{-1}(x) + \lambda\theta(1-x)$.

From its definition (6.2), and using (5.16) for the normalization, one obtains

$$\alpha = \tfrac{1}{2}(K \tanh K - \sinh^2 K). \tag{6.9}$$

If $\lambda > 0$ the frequency shifts $\pm\sqrt{\lambda\alpha}$ are purely imaginary, while for $\lambda < 0$ they are real. That is, as λ is turned from positive through zero to negative values, the complex poles move together horizontally, merge, and then move apart vertically; cf section 3.1.

Proceeding to $\mathcal{O}(\lambda)$, conventional QNM perturbation theory [15] gives the coefficients of the shift as $\langle \tilde{\boldsymbol{f}}^0_{(0)} | \tilde{H}' \tilde{\boldsymbol{f}}^{(0)}_0 \rangle / \langle \tilde{\boldsymbol{f}}^0_{(0)} | \tilde{\boldsymbol{f}}^{(0)}_0 \rangle$ and $\langle \tilde{\boldsymbol{f}}^0_{(1)} | \tilde{H}' \tilde{\boldsymbol{f}}^{(1)}_0 \rangle / \langle \tilde{\boldsymbol{f}}^0_{(1)} | \tilde{\boldsymbol{f}}^{(1)}_0 \rangle$, respectively[9]. Using (6.7), both are evaluated as $\frac{1}{2}(H'_{00} + H'_{11}) + \mathcal{O}(\sqrt{\lambda}) = H'_{00} + \mathcal{O}(\sqrt{\lambda})$, where the last step follows from the symmetry pointed out below (6.8). In the numerator of

$$H'_{00} = \frac{(\boldsymbol{f}_{0,1},\, H' \boldsymbol{f}_0)}{(\boldsymbol{f}_{0,1},\, \boldsymbol{f}_0)} \tag{6.10}$$

the contribution of f_b as in (5.15c) (i.e., the term found only by proper bi-orthogonalization which does not contribute to the denominator in (6.10), cf below (5.16)) is seen to be $\propto \alpha$ upon comparison with (6.2). For both split levels the next-order shift thus reads

$$\begin{aligned} \lambda H'_{00} &= \lambda \left[\frac{(\boldsymbol{f}_a,\, H' \boldsymbol{f}_0)}{(\boldsymbol{f}_{0,1},\, \boldsymbol{f}_0)} - \mathrm{i} \left(\frac{2}{3} \frac{K}{\gamma} + \frac{1}{2K} \right) \tanh(K) \alpha \right] \\ &= \mathrm{i} \frac{\lambda}{\gamma} \left(\frac{K}{4} \tanh K - \frac{K}{6} \frac{\sinh^3 K}{\cosh K} - \frac{K^2}{4} - \frac{K^2}{12} \tanh^2 K \right) \end{aligned} \tag{6.11}$$

and is imaginary, so that if the double pole is split along the imaginary axis in $\mathcal{O}(\lambda^{1/2})$ the QNMs stay on this axis up to $\mathcal{O}(\lambda)$, again consistent with the argument of section 3.1.

For a check, the perturbed QNMs can be also found directly from (2.2) together with the boundary conditions. For a constant $\rho'(0<x<a)^{-1} = \gamma^2/K^2 + \lambda$, the eigenvalue equation is

$$\mathrm{i} - \sqrt{\rho'} \operatorname{cotan}(\sqrt{\rho'}\omega) = -\omega \frac{K^2}{\gamma^2 \sinh^2 K} \tag{6.12}$$

[15] Strictly speaking, ρ^{-1} is undefined if ρ contains a δ-function as in (3.5c). This can be dealt with as a limiting case of regular ρ. To be sure, no problems arise here.

in which we set $\sqrt{\rho'} = K/\gamma - (K^3/2\gamma^3)\lambda + \mathcal{O}(\lambda^2)$ and $\omega = -\mathrm{i}\gamma + \omega_1\sqrt{\lambda} + \omega_2\lambda + \omega_3\lambda^{3/2} + \mathcal{O}(\lambda^2)$. In $\mathcal{O}(\lambda^0)$ and $\mathcal{O}(\sqrt{\lambda})$, (6.12) is satisfied identically. In $\mathcal{O}(\lambda)$ one obtains $\omega_1^2 = \alpha$, with α as in (6.9); in $\mathcal{O}(\lambda^{3/2})$ one obtains $\omega_2 = H'_{00}$, with H'_{00} as in (6.11). Hence, the Jordan-block BB formalism of section 6.1 agrees with direct expansion of the wave equation.

Finally, non-generic perturbations are illustrated by $K \mapsto K' = K + \lambda$ in (3.5*c*), namely by $\delta\rho = \partial_K \rho$ (in the differentiation of ρ, its K-dependence through γ as in (3.5*b*) must also be taken into account). In the lowest order, H' shifts the double pole corresponding to K to a double pole for K', and indeed one finds $\int_0^{1^+} \delta\rho f_0^2 \,\mathrm{d}x = 0$, as stipulated below (6.3). Since beyond this leading order $H_0(K) + \lambda H' \neq H_0(K')$, the double pole will be split eventually. In line with section 6.1, however, this is not pursued here.

7. Conclusion

A remark is in place concerning the *relevance* of the issue considered. The preceding and especially section 6 make clear that non-trivial Jordan blocks occur only on a set of measure zero in parameter space. However, this feature is shared with, e.g., stationary points in the phase space of dynamical systems, critical points in phase diagrams (note the semantic coincidence with 'critical damping'), and degeneracies in conservative quantum systems. All of these are worthy of study and to a remarkably large extent determine the global structure of the parameter space. For degenerate quantum levels, a further motivation is their relation to symmetry. While no analogue has shown up here, two modes *can* merge in a spatially symmetric open wave system's superpartner [31].

The existence questions raised in section 3 and appendix A are related to *spectral inversion*. In the closed case, the classic inverse problem [32] is to determine the system ($\rho(x)$ for the wave equation or $V(x)$ for the Klein–Gordon equation) given all real eigenfrequencies ω_j. The counterpart for open systems is to find ρ or V from the *complex* ω_j or, more generally, from the singularities of $\tilde{G}(\omega)$. If, e.g., $\tilde{G}$ is specified to have a pole of order $M_j = 4$ at ω_j, does a corresponding ρ or V exist (at least for one in a class of such singularity configurations)? Assuming the general inverse problem for open systems (a topic for further research) to be tractable, at this stage the following scenarios are conceivable.

(i) The inversion algorithm indeed yields a ρ with, say, a fourth-order pole or a pair of off-axis double poles in its spectrum.
(ii) The inverse problem turns out to have no solutions, yielding a non-trivial proof of the non-existence of such configurations.
(iii) This particular set of singularities points to limitations in the inversion algorithm which otherwise might have been overlooked.

Any of these would further the understanding of QNMs in open wave systems.

As mentioned in section 1, for the case of simple poles we have second-quantized the open wave system (2.1) using QNMs [13]. The expansion coefficients a_j (cf (2.12)) emerge as the pertinent quantum degrees of freedom, in terms of which it is possible to eliminate the outside from the equations for the cavity evolution. This relevance to the quantum problem further motivates studying the mode structure of (2.1). The present groundwork indeed facilitates second quantization even when this structure involves non-trivial Jordan blocks, either by Hilbert-space methods or by exactly solving the associated path integral [14].

In closing, it may be useful to place this paper into the following context. Many wave phenomena obey an evolution equation $\mathrm{i}\partial_t\phi = H\phi$ (see above (2.4)) and a logical question is: what are the possible forms for H—leading to various dynamics for ϕ—and how are these exemplified in nature? The most familiar are conservative systems, for which ϕ is

expandable in a complete normal-mode basis, diagonalizing H, with real eigenvalues. Our earlier work [9, 12] shows another realization: in a large class of outgoing-wave systems, ϕ is again expandable in a complete basis (of QNMs) in terms of which H again is diagonal, but with complex eigenvalues. The QNMs, however, are not orthogonal under the standard inner product. Therefore it is convenient to introduce their duals as well; together these constitute a BB. This paper has identified and studied a further generalization pertaining to such open wave systems, for which H is not diagonalizable. In these circumstances we have shown that a well-defined Jordan-block structure emerges, involving a non-trivial duality operator.

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Appendix A. Third-order poles and beyond

At present, it is not known whether higher-order poles can exist off the imaginary axis, cf section 3.1. The analogy to damped harmonic oscillators suggests that they cannot, but this does not lead to a proof directly since the oscillator picture itself is contingent on the QNM spectrum being simple, with at most a double-pole zero-mode. In fact, at the end of section 3.2 it was pointed out that the analogy is imperfect, and also intuition based on the conservative and WKB limits could bias one against more exotic possibilities.

A possible strategy for looking for off-axis double poles is to first construct a fourth-order zero-mode, which under a suitable non-generic perturbation could be split into a pair of such double poles, cf section 6.2. Thus returning to the case $\omega = -\mathrm{i}\gamma$, (5.13) shows that for a fourth-order pole one needs[9] $(\boldsymbol{f}_0, \boldsymbol{f}_{0,1}) = (\boldsymbol{f}_{0,1}, \boldsymbol{f}_{0,1}) = 0$. Expanding $f_{0,1}$ by its integral representation[11], using (4.4) for its momentum, and eliminating ρ and γ by (3.1) and (3.3) respectively, one arrives at two functional equations for[16] $f_0 = f$

$$\gamma^2 W_{0,2} = 4\int_0^1 \frac{\mathrm{d}x}{f^2(x)}\left[\int_0^x \mathrm{d}y\, f''(y)f(y)\right]^2 - \int_0^1 (f')^2\,\mathrm{d}x = 0 \tag{A.1}$$

$$\mathrm{i}\gamma^3 W_{0,3} = 8\int_0^1 \mathrm{d}x\, f''(x)f(x)\left[\int_x^1 \frac{\mathrm{d}y}{f^2(y)}\int_0^y \mathrm{d}z\, f''(z)f(z)\right]^2 - 4\int_0^1 \frac{\mathrm{d}x}{f^2(x)}\left[\int_0^x \mathrm{d}y\, f''(y)f(y)\right]^2 = 0 \tag{A.2}$$

where $a \equiv 1$ without loss of generality; (A.1) alone yields a third-order pole. Solutions are to be sought among the f satisfying conditions (a) below (3.3) and the inequality (3.4).

Up to now we have only studied third-order poles, seeking f obeying (A.1) and subsequently constructing ρ using (3.1). We have considered $f(x) = x + \alpha x^n$ $(n > 2)$, cf below (3.4)[17]. One has $W_{0,2} < 0$ both for small and for large α: (a) for small α, $f'' \approx 0$ so that the second term in (A.1) dominates; (b) for large α, one can neglect the linear term to find that $\gamma^2 W_{0,2} = -\alpha^2 n^2(4n-3)/(2n-1)^3 < 0$. However, there exist n for which $W_{0,2} > 0$ if $\alpha \in (\alpha_1, \alpha_2)$—so $W_{0,2} = 0$ at α_1 and at α_2—e.g., $(\alpha_1, \alpha_2) = (2.059, 3.8209)$ for $n = 5$, and $(\alpha_1, \alpha_2) = (1.063\,096, 8.309\,08)$ for $n = 6$. In both cases, (3.4) is violated at α_1 but

[16] In further numerical work, one should circumvent the time-consuming multiple integrals in (A.1) and (A.2). For instance, $p = 4\int_0^1 \mathrm{d}x\, f^{-2}(x)[\int_0^x \mathrm{d}y\, f''(y)f(y)]^2$ is the solution $p(1)$ of the system $\{(p,q)' = (4q^2/f^2, f''f),\ (p(0), q(0)) = (0,0)\}$.

[17] In this example, $\rho(x) \to 0$ if $x \to 0$ and $n > 3$, but this can always be remedied by adding a small positive x^3 term and adjusting α accordingly.

satisfied at α_2, implying that third-order poles indeed do exist. Besides being a stepping-stone in the search for fourth-order (and hence off-axis) poles, this result in itself already justifies the general (i.e., not limited to $M_j \leqslant 2$) setup in sections 4–6.

Appendix B. Constructing dual bases

In section 5, one needs to determine the basis dual to $\{\boldsymbol{f}_{j,n}\}_{n=0}^{M_j-1}$. There is a standard result for finite-dimensional spaces [16], which, however, applies for a dual basis constructed *within* the space spanned by the original one. Here we are concerned with the original space $V = \mathcal{L}[\{\boldsymbol{f}_{j,n}\}_{n=0}^{M_j-1}]$ ($\mathcal{L}$ is the linear span), but with the dual basis in a *different* space W.

Therefore we are led to the following problem. Let V be an M-dimensional subspace of a Hilbert space with basis $\{v_n\}_{n=0}^{M-1}$, and let W be another M-dimensional subspace of the same Hilbert space. Under what conditions will there be a dual basis $\{w^n\}$ in W, in the sense that $\langle w^m|v_n\rangle = \delta_{mn}$? We claim that the necessary and sufficient condition is

$$W \cap V^{\perp} = \{0\} \tag{B.1}$$

where $V^{\perp}$ is the orthogonal complement to V. (For example, if the whole Hilbert space is three dimensional, and if V is the x–y plane, then W must not contain the z-axis.)

For a proof, let $\{w_n\}$ be any basis for W. The duality of $\{w^n\}$ and $\{v_n\}$ is equivalent to

$$\begin{pmatrix} \langle w_0|v_0\rangle & \cdots & \langle w_0|v_{M-1}\rangle \\ \vdots & & \vdots \\ \langle w_{M-1}|v_0\rangle & \cdots & \langle w_{M-1}|v_{M-1}\rangle \end{pmatrix} \begin{pmatrix} w^0 \\ \vdots \\ w^{M-1} \end{pmatrix} = \begin{pmatrix} w_0 \\ \vdots \\ w_{M-1} \end{pmatrix}. \tag{B.2}$$

The solvability condition is that the metric matrix on the LHS be non-singular. Singularity would mean that a non-trivial linear superposition w of the w_m (i.e., a non-zero vector in W) is perpendicular to all v_n, i.e., that $w \in V^{\perp}$. This simple calculation not only proves our assertion, but also gives a constructive algorithm.

Returning to the outgoing-wave system of the main text, the contour-integral calculation there in effect shows that (B.1) is indeed satisfied for $V_j = \mathcal{L}[\{\boldsymbol{f}_{j,n}\}_{n=0}^{M_j-1}]$ and $W_j = \mathcal{F}V_j$ with $\mathcal{F}$ as in (2.14), solves (B.2) for that case, and extends this bi-orthogonalization to the whole space by showing that the latter equals $\oplus_j V_j$, with (4.6) holding between different blocks.

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