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Resolvent expansion for discrete non-Hermitian resonant systems [Invited]

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Abstract: The linear response of non-Hermitian resonant systems demonstrates various intriguing features such as the emergence of non-Lorentzian lineshapes. Recently, we have developed a systematic theory to understand the scattering lineshapes in such systems and, in doing so, established the connection with the input/output scattering channels. Here, we follow up on that work by presenting a different, more transparent derivation of the resolvent operator associated with a non-Hermitian system under general conditions and highlight the connection with the structure of the underlying eigenspace decomposition. Finally, we also present a simple solution to the problem of self-orthogonality associated with the left and right Jordan canonical vectors and show how the left basis can be constructed in a systematic fashion. Our work provides a unifying mathematical framework for studying non-Hermitian systems such as those implemented using dielectric cavities, metamaterials, and plasmonic resonators.

1. Introduction

Over the last few years, the physics of non-Hermitian systems has attracted considerable attention and inspired numerous studies that explore its implications using various platforms such as optics [1–3], electronics [4–6], and acoustics [7,8]. In these efforts, the spectral response of the relevant system was obtained by using direct calculations of the various scattering coefficients. While this strategy is successful for small systems having few modes, it can be tedious for larger systems with many degrees of freedom. In addition, it does not provide any insight into the response function. Recently, we have developed a general linear response theory for discrete non-Hermitian systems (coupled optical microresonators or electronic circuits for example) having exceptional points (EPs) [9]. In that work, we derived a closed form solution for the resolvent operator (sometimes called the Green's function) expansion in terms of the system's eigenvectors and the Jordan canonical vectors. This expansion provides a systematic explanation for the structure of the spectral response and particularly the presence of higher-order Lorentzian lineshapes and their dependence on the input and output channels. Importantly, the resolvent expansion in our earlier work is valid for any generic system having any number of EPs of any order and for any excitation profile and frequency. Our derivation in [9] relies on the algebra of the eigenvectors and the canonical vectors (bi-orthogonality, self-orthogonality, etc.) associated with the underlying

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Hamiltonian. While this strategy is technically successful, it does not necessarily emphasize the connection between the resolvent expansion and the structure of the eigenspace.

In this work, we present an alternative, more transparent derivation of the resolvent operator associated with a generic, discrete non-Hermitian system that highlights the structure of the eigenspace and also establishes the connection with prior works that focused only on the special, more restrictive scenario of a non-Hermitian system in the vicinity of EPs. In addition, we also present a straightforward solution to the problem of self-orthogonality associated with the Jordan canonical vectors, which in turn facilitates the evaluation of the linear response of non-Hermitian systems.

2. Results

Resolvent expansion:— Similar to our work in [9], we start by considering a linear, discrete system (see Fig. 1) described by a set of coupled ordinary differential equations of the form:

$$i\frac{d|a(t)\rangle}{dt} = H|a(t)\rangle + i\Gamma|b(t)\rangle, \tag{1}$$

where the kets $|a(t)\rangle = [a_1(t), a_2(t), \dots, a_N(t)]^T$, $|b(t)\rangle = [b_1(t), b_2(t), \dots, b_L(t)]^T$ represent the field amplitudes inside the discrete system (the electric fields inside coupled optical resonators as an example) and the excitation signal, respectively. In addition, the $N \times N$ matrix H describes the interaction between the excitation amplitudes associated with the individual resonant elements of the system while Γ is the $N \times L$ coupling matrix between L input channels and the excitation amplitudes. This system of equations can model coupled optical, electronic, acoustic, or mechanical systems (see Fig. 1). In some situations, such as in optics, the above equation is also supplemented by an output relation of the form $|v(t)\rangle = \hat{Y}|b(t)\rangle - \Gamma^T|a(t)\rangle$, where $|v(t)\rangle = [v_1(t), v_2(t), \dots, v_L(t)]^T$ are the output field amplitudes, and $\hat{Y}$ describes the the direct coupling between the input and output channels. Following [9], we will simplify the notation and define $|f(t)\rangle = i\Gamma|b(t)\rangle$. Expressed in the Fourier domain (defined in the bases $e^{-i\omega t}$) Eq. (1) takes the form $(\omega I - H)|A(\omega)\rangle = |F(\omega)\rangle$, which admits the solution:

$$|A(\omega)\rangle = G(\omega)|F(\omega)\rangle, \tag{2}$$

with $G(\omega) \equiv (\omega I - H)^{-1}$.

The goal of this paper is to derive an expression for $G(\omega)$ in terms of the eigenvectors and canonical vectors of H under general conditions. In what follows, we suppress the dependence on ω but keep in mind that we are working in the Fourier domain. Without loss of generality, we assume that the spectrum of the Hamiltonian H exhibits $N - M$ distinct eigenvalues and one EP of order M (the order of an EP defines the number of coalescing eigenstates forming the EP) defined by $(H - \omega_n I)|\phi_n^r\rangle = 0$, for $n = 1, 2, .., N - M$, and $(H - \omega_{\mathrm{EP}} I)|\phi_{\mathrm{EP}}^r\rangle = 0$. Here, the subscript r refers to right eigenvectors as opposed to left eigenvectors which we will define below. Obviously, the eigenvectors of H do not span the whole underlying space. It is well known, however, that the underlying space can be completed by using the Jordan canonical vectors defined as $(H - \omega_{\mathrm{EP}} I)|J_m^r\rangle = \chi_m|J_{m-1}^r\rangle$, for $m = 1, \dots, M$. Here, we define $|J_1^r\rangle \equiv |\phi_{\mathrm{EP}}^r\rangle$ which satisfies $(H - \omega_{\mathrm{EP}} I)|J_1^r\rangle = 0$, and the constants χ_m are introduced to ensure that the physical dimensions remain consistent with their numerical values chosen such that $\langle J_m^r | J_m^r \rangle = 1$. Due to the non-Hermiticity of H, the eigenvectors $|\phi_n^r\rangle$ are not orthogonal. However, the left and right eigenvectors satisfy the bi-orthogonality condition $\langle \phi_m^l | \phi_n^r \rangle = \delta_{m,n}$ with the left eigenvectors defined as $\langle \phi_n^l | (\omega I - H) = 0$. This, however, is not necessarily the case for the Jordan canonical vectors since some of them may be self-orthogonal, i.e. $\langle J_m^l | J_m^r \rangle = 0$ for some values of m (see Supplementary Note 2 in [9]). In our previous work [9], we did not present an algorithmic solution to this problem. Instead, we considered generalized left vectors $\langle \tilde{J}_m^l|$ that satisfy the relation

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$\langle \tilde{J}_m^l | J_n^r \rangle = \delta_{m,n}$. Such generalized vectors can be constructed by applying an orthogonalization technique (for instance, the Gram-Schmidt procedure [10]) to the left canonical vectors. In the main text here, we will use the same notation but will present a straightforward algorithmic strategy for building this bi-orthogonal set shortly after. In contrast to our work in [9], where a general expansion was sought after directly, here we proceed by decomposing the full space $\mathcal{U}$ into manifolds $\mathcal{U}^{\mathrm{w,v}}$, i.e. $\mathcal{U} = \mathcal{U}^{\mathrm{w}} \bigoplus \mathcal{U}^{\mathrm{v}}$ with $\bigoplus$ denoting the direct sum (see Fig. 2). The key property of $\mathcal{U}^{\mathrm{w,v}}$ is their invariance under the action of the Hamiltonian H. Here, $\mathcal{U}^{\mathrm{w}}$ is an invariant subspace spanned by the set of all the right eigenvectors $|\phi_n^r\rangle$ except the exceptional vector $|J_1^r\rangle$, while $\mathcal{U}^{\mathrm{v}}$ is an invariant subspace spanned by the right exceptional vector together with the right Jordan vectors $|J_m^r\rangle$ for $m \geq 2$ (see Supplementary Note 1 for more discussion on this decomposition).

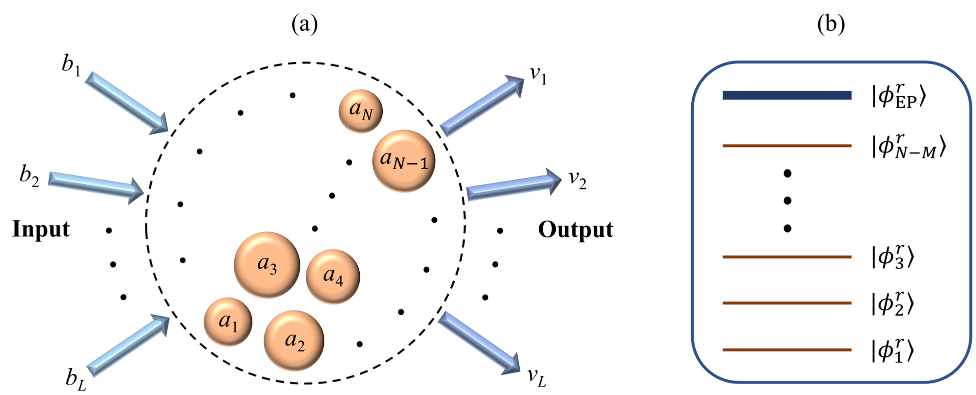

Fig. 1. Illustration of the system and its underlying properties. (a) A schematic of a discrete non-Hermitian system made of N coupled resonators and having multiple input b_m and output v_m channels. The field amplitude in resonator n is denoted by a_n. (b) An illustration of one possible scenario for the spectrum associated with the underlying Hamiltonian of the structure in (a). In that particular example, the system has $N - M$ distinct eigenstates associated with the eigenvectors $|\phi_n^r\rangle$ and an exceptional point of order M corresponding to an exceptional vector $|\phi_{\mathrm{EP}}^r\rangle$. The analysis presented in this work is general and applies to any other scenario.

It is well known that under the above space decomposition, there exists a similarity transformation that casts the matrix Hamiltonian H in the block diagonal form $H = \begin{pmatrix} H^{\mathrm{w}} & 0_{12} \\ 0_{21} & H^{\mathrm{v}} \end{pmatrix}$, where $H^{\mathrm{w,v}}$ are $(N-M) \times (N-M)$ and $M \times M$ block matrices, respectively; and 0_{12} is a $(N-M) \times M$ null matrix with 0_{21} being the transpose of 0_{12}. In this basis, any vector $|u\rangle$ can be naturally partitioned into two components $|u\rangle = \begin{pmatrix} |u^{\mathrm{w}}\rangle \\ |u^{\mathrm{v}}\rangle \end{pmatrix}$ where $|u^{\mathrm{w}}\rangle$ is an $N - M$ dimensional vector that spans $\mathcal{U}^{\mathrm{w}}$ while $|u^{\mathrm{v}}\rangle$ is an M dimensional vector that spans $\mathcal{U}^{\mathrm{v}}$. Importantly, in this basis, the eigenvectors and canonical vectors take the form $|\phi_n^r\rangle = \begin{pmatrix} |\phi_n^{\mathrm{w},r}\rangle \\ |0^{\mathrm{v}}\rangle \end{pmatrix}$ and $|J_m^r\rangle = \begin{pmatrix} |0^{\mathrm{w}}\rangle \\ |J_m^{\mathrm{v},r}\rangle \end{pmatrix}$. By using this decomposition scheme, one can now express the resolvent operator and the spectral

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responses in the form $G(\omega) \equiv (\omega I - H)^{-1} = \begin{pmatrix} G^{\mathrm{w}}(\omega) & 0_{12} \\ 0_{21} & G^{\mathrm{v}}(\omega) \end{pmatrix}$ and $|A^{\mathrm{w,v}}\rangle = G^{\mathrm{w,v}}|F^{\mathrm{w,v}}\rangle$ where $G^{\mathrm{w,v}}(\omega) = (\omega I - H^{\mathrm{w,v}})^{-1}$, $|A\rangle = \begin{pmatrix} |A^{\mathrm{w}}\rangle \\ |A^{\mathrm{v}}\rangle \end{pmatrix}$, and $|F\rangle = \begin{pmatrix} |F^{\mathrm{w}}\rangle \\ |F^{\mathrm{v}}\rangle \end{pmatrix}$.

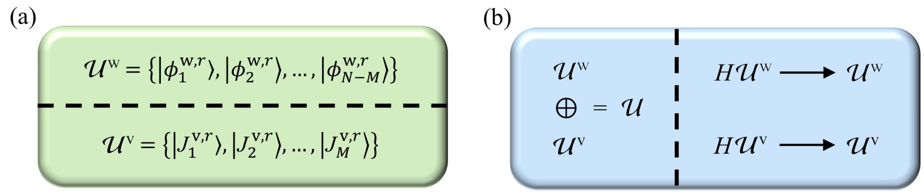

Fig. 2. Structure of the eigenspace associated with the Hamiltonian H. (a) The construction of the subspaces $\mathcal{U}^{\mathrm{w}}$ and $\mathcal{U}^{\mathrm{v}}$ in terms of the right eigenvectors, the exceptional vector, and the Jordan vectors. (b) Illustration of the decomposition properties of $\mathcal{U}$ into the subspaces $\mathcal{U}^{\mathrm{w,v}}$ and the invariance of the latter under the action of the Hamiltonian H.

The above discussion demonstrates that the task of finding the Green's operator over the complete space can be eventually reduced to evaluating the Green's operators over the two subspaces $\mathcal{U}^{\mathrm{w,v}}$ independently which greatly simplifies the analysis. In particular, for the subspace $\mathcal{U}^{\mathrm{w}}$ spanned by $|\phi_n^{\mathrm{w},r}\rangle$, we find that:

$$G^{\mathrm{w}}(\omega) = \sum_{n=1}^{N-M} \frac{|\phi_n^{\mathrm{w},r}\rangle\langle\phi_n^{\mathrm{w},l}|}{\omega - \omega_n}. \tag{3}$$

This expression can be obtained by simply invoking the completeness relation of the identity operator associated with $\mathcal{U}^{\mathrm{w}}$: $I^{\mathrm{w}} = \sum_{n=1}^{N-M} |\phi_n^{\mathrm{w},r}\rangle\langle\phi_n^{\mathrm{w},l}|$ in conjunction with $|A^{\mathrm{w}}\rangle = G^{\mathrm{w}}|F^{\mathrm{w}}\rangle$ (see Supplementary Note 2).

On the other hand, for the subspace $\mathcal{U}^{\mathrm{v}}$, the expression for the Green's operator in terms of the Hamiltonian is given by:

$$G^{\mathrm{v}}(\omega) = \sum_{k=1}^{M} \frac{(H^{\mathrm{v}} - \omega_{\mathrm{EP}} I)^{k-1}}{(\omega - \omega_{\mathrm{EP}})^k}. \tag{4}$$

This series expansion in terms of H is discussed in [11–13]. A particularly elegant and more transparent derivation of this expansion that makes use of the nilpotent nature of the matrix $(H^{\mathrm{v}} - \omega_{\mathrm{EP}} I)$ has been recently presented in [14], which we also reproduce in Supplementary Note 3 for completeness.

Again, by invoking the identity operator associated with subspace $\mathcal{U}^{\mathrm{v}}$, namely $I^{v} = \sum_{k=1}^{M} |J_k^{\mathrm{v},r}\rangle\langle\tilde{J}_k^{\mathrm{v},l}|$, we obtain:

$$G^{\mathrm{v}}(\omega) = \sum_{k=1}^{M} \frac{|J_k^{\mathrm{v},r}\rangle\langle\tilde{J}_k^{\mathrm{v},l}|}{\omega - \omega_{\mathrm{EP}}} + \sum_{k=2}^{M} \frac{\chi_k |J_{k-1}^{\mathrm{v},r}\rangle\langle\tilde{J}_k^{\mathrm{v},l}|}{(\omega - \omega_{\mathrm{EP}})^2} + \sum_{k=3}^{M} \frac{\chi_k \chi_{k-1} |J_{k-2}^{\mathrm{v},r}\rangle\langle\tilde{J}_k^{\mathrm{v},l}|}{(\omega - \omega_{\mathrm{EP}})^3} + \cdots \tag{5}$$

which we can cast in the form:

$$G^{\mathrm{v}}(\omega) = \sum_{m=1}^{M} \sum_{k=m}^{M} \alpha_k^{(m)} \frac{|J_m^{\mathrm{v},r}\rangle\langle\tilde{J}_k^{\mathrm{v},l}|}{(\omega - \omega_{\mathrm{EP}})^{k-m+1}}, \tag{6}$$

with the coefficients $\alpha_k^{(m)}$ given by $\alpha_m^{(m)} = 1$ and $\alpha_k^{(m)} = \alpha_{k-1}^{(m)} \chi_k$ (see Supplementary Note 3).

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Therefore, the resolvent operator is given by:

$$G(\omega) = \begin{pmatrix} \sum_{n=1}^{N-M} \frac{|\phi_n^{\mathrm{w},r}\rangle\langle\phi_n^{\mathrm{w},l}|}{\omega-\omega_n} & 0_{12} \\ 0_{21} & \sum_{m=1}^{M}\sum_{k=m}^{M} \alpha_k^{(m)} \frac{|J_m^{\mathrm{v},r}\rangle\langle\tilde{J}_k^{\mathrm{v},l}|}{(\omega-\omega_{\mathrm{EP}})^{k-m+1}} \end{pmatrix}. \tag{7}$$

Note that the above expansion is expressed in terms $|\phi_n^{\mathrm{w},r}\rangle$ and $|J_m^{\mathrm{v},r}\rangle$ together with the corresponding left vectors. Our goal, however, is to express $G(\omega)$ in terms of the vectors associated with the full space, i.e. $|\phi_n^r\rangle$ and $|J_m^r\rangle$. To do so, we first recall the definition $|\phi_n^r\rangle = \begin{pmatrix} |\phi_n^{\mathrm{w},r}\rangle \\ |0^{\mathrm{v}}\rangle \end{pmatrix}$. It is then straightforward to show that:

$$\sum_{n=1}^{N-M} \frac{|\phi_n^r\rangle\langle\phi_n^l|}{\omega-\omega_n} = \begin{pmatrix} \sum_{n=1}^{N-M} \frac{|\phi_n^{\mathrm{w},r}\rangle\langle\phi_n^{\mathrm{w},l}|}{\omega-\omega_n} & 0_{12} \\ 0_{21} & 0_{22} \end{pmatrix}, \tag{8}$$

where here 0_{22} is a $M \times M$ null matrix.

Similarly, by recalling that $|J_m^r\rangle = \begin{pmatrix} |0^{\mathrm{w}}\rangle \\ |J_m^{\mathrm{v},r}\rangle \end{pmatrix}$, we find that:

$$\sum_{m=1}^{M}\sum_{k=m}^{M} \alpha_k^{(m)} \frac{|J_m^r\rangle\langle\tilde{J}_k^l|}{(\omega-\omega_{\mathrm{EP}})^{k-m+1}} = \begin{pmatrix} 0_{11} & 0_{12} \\ 0_{21} & \sum_{m=1}^{M}\sum_{k=m}^{M} \alpha_k^{(m)} \frac{|J_m^{\mathrm{v},r}\rangle\langle\tilde{J}_k^{\mathrm{v},l}|}{(\omega-\omega_{\mathrm{EP}})^{k-m+1}} \end{pmatrix}, \tag{9}$$

where here 0_{11} is a $(N-M)\times(N-M)$ null matrix.

By adding the two expressions in Eqs. (8) and (9), we arrive at:

$$\begin{aligned} &\sum_{n=1}^{N-M} \frac{|\phi_n^r\rangle\langle\phi_n^l|}{\omega-\omega_n} + \sum_{m=1}^{M}\sum_{k=m}^{M} \alpha_k^{(m)} \frac{|J_m^r\rangle\langle\tilde{J}_k^l|}{(\omega-\omega_{\mathrm{EP}})^{k-m+1}} = \\ &\begin{pmatrix} \sum_{n=1}^{N-M} \frac{|\phi_n^{\mathrm{w},r}\rangle\langle\phi_n^{\mathrm{w},l}|}{\omega-\omega_n} & 0_{12} \\ 0_{21} & \sum_{m=1}^{M}\sum_{k=m}^{M} \alpha_k^{(m)} \frac{|J_m^{\mathrm{v},r}\rangle\langle\tilde{J}_k^{\mathrm{v},l}|}{(\omega-\omega_{\mathrm{EP}})^{k-m+1}} \end{pmatrix}. \end{aligned} \tag{10}$$

The RHS of Eq. (10) is $G(\omega)$, so we finally obtain:

$$G(\omega) = \sum_{n=1}^{N-M} \frac{|\phi_n^r\rangle\langle\phi_n^l|}{\omega-\omega_n} + \sum_{m=1}^{M}\sum_{k=m}^{M} \alpha_k^{(m)} \frac{|J_m^r\rangle\langle\tilde{J}_k^l|}{(\omega-\omega_{\mathrm{EP}})^{k-m+1}}. \tag{11}$$

The above expression is exactly the result obtained in our earlier work [9]. While the result here is derived in a particular basis, it is straightforward to check that the mathematical structure of the above expression is invariant under similarity transformations (see Supplementary Note 4).

Left vector basis:— From the definition of the left eigenvectors $\langle\phi_n^l|$, it is obvious that they are unique and can be found by solving a row eigenvalue problem (as opposed to the standard column eigenvalue problem associated with right eigenvectors). However, as indicated above and discussed in detail in [9], the situation is more complicated for the canonical vectors since some of them are self-orthogonal, i.e. they can satisfy $\langle J_m^l|J_m^r\rangle = 0$ for some values of m. In the main text, we assumed that we have obtained, somehow, a set of left vectors that together with the right canonical vectors form a bi-orthogonal set. Here, we present a straightforward procedure to obtain such a set and, in doing so, we also obtain the left eigenvectors automatically without

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solving any eigenvalue problem. To do so, we first note that the set of right eigenvectors $\{|\phi_n^r\rangle\}$ and right canonical vectors $\{|J_m^r\rangle\}$ are linearly independent [9]. We now form the matrix Q_1 whose columns are exactly these vectors, i.e. $Q_1 = [|\phi_1^r\rangle \cdots |\phi_{N-M}^r\rangle, |J_1^r\rangle \cdots |J_M^r\rangle]$. Let us now assume that we have found the set of the left vectors $\{\langle\phi_n^l|\}$ and $\{\langle\tilde{J}_n^l|\}$. Each of these vectors is orthogonal to all the different right vectors and has a finite projection on the corresponding right vectors which can be chosen to be unity, i.e. there is no self-orthogonality. If we arrange these left vectors as the rows in matrix Q_2 according to $Q_2 = [|\phi_1^l\rangle \cdots |\phi_{N-M}^l\rangle, |\tilde{J}_1^{\,l}\rangle \cdots |\tilde{J}_M^{\,l}\rangle]^\dagger$, where the superscript † indicates Hermitian conjugation, and invoke the bi-orthogonality, we obtain $Q_2 Q_1 = I$, where I is the identity matrix. In other words, we have $Q_2 = Q_1^{-1}$. Thus, once the right eigenvectors and canonical vectors are obtained, the bi-orthogonal left vectors can be determined by a simple matrix inversion.

Working example:— We illustrate here the above results by presenting a simple example for calculating the right/left vectors and the Green's operator in a different basis. To do so, we consider the following Hamiltonian matrix $H = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 0 & 2 \end{pmatrix}$, which is already in the Jordan canonical form. The eigenvalues of H are $\lambda_1 = 1$ and $\lambda_{2,3} = 2$. The first eigenvalue corresponds to a distinct eigenvector $|\phi_1^r\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, whereas $\lambda_{2,3}$ is associated with an EP of order two and an exceptional vector given by $|\phi_{\text{EP}}^r\rangle \equiv |J_1^r\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$. The right Jordan canonical vectors can be easily obtained from its definition. Choosing $\chi_2 = 1$, we find $|J_2^r\rangle = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$.

In order to calculate the left vectors, we apply the procedure outlined above, i.e. we construct the matrix $Q_1 = [|\phi_1^r\rangle, |J_1^r\rangle, |J_2^r\rangle] = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}$ and calculate its inversion, $Q_2 = [|\phi_1^l\rangle, |\tilde{J}_1^{\,l}\rangle, |\tilde{J}_2^{\,l}\rangle]^\dagger = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{pmatrix}$. The left bi-orthogonal set of vectors can be then read off immediately as $\langle\phi_1^l| = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix}$, $\langle\tilde{J}_1^l| = \begin{pmatrix} 0 & 1 & -1 \end{pmatrix}$, and $\langle\tilde{J}_2^l| = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix}$.

By substituting these results directly in Eq. (11), we obtain:

$$G(\omega) = \frac{|\phi_1^r\rangle\langle\phi_1^l|}{\omega - 1} + \frac{|J_1^r\rangle\langle\tilde{J}_1^l|}{\omega - 2} + \frac{|J_1^r\rangle\langle\tilde{J}_2^l|}{(\omega - 2)^2} + \frac{|J_2^r\rangle\langle\tilde{J}_2^l|}{\omega - 2} = \begin{pmatrix} \frac{1}{\omega-1} & 0 & 0 \\ 0 & \frac{1}{\omega-2} & \frac{1}{(\omega-2)^2} \\ 0 & 0 & \frac{1}{\omega-2} \end{pmatrix}. \tag{12}$$

Note that the matrix form of $G(\omega)$ is in accordance with what one would expect for a Hamiltonian H that is already in the Jordan canonical form.

Let us now consider the non-trivial case of a Hamiltonian that is not in its Jordan form. For sake of simplicity, we will consider the same H as before but written in different basis via a similarity transform $H_{\text{new}} = T^{-1}HT$. Here, we will choose $T = \begin{pmatrix} 1 & 1 & 2 \\ 0 & 2 & 3 \\ 0 & 1 & 2 \end{pmatrix}$, which gives:

$$H_{\text{new}} = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & -3 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} 1 & 1 & 2 \\ 0 & 2 & 3 \\ 0 & 1 & 2 \end{pmatrix} = \begin{pmatrix} 1 & -1 & -2 \\ 0 & 4 & 4 \\ 0 & -1 & 0 \end{pmatrix}. \tag{13}$$

By repeating the same procedure as above, we find that the distinct eigenvector to be $|\psi_1^r\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ while the exceptional vector and Jordan vector are $|h_1^r\rangle = \begin{pmatrix} 0 \\ -2 \\ 1 \end{pmatrix}$ and $|h_2^r\rangle = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$ (obtained for $\chi_2 = 1$ as before), respectively. The left bi-orthogonal vectors can be easily obtained as before by evaluating Q_1 and its inverse $Q_2 = \begin{pmatrix} 1 & 0 & 1 \\ 0 & -2 & -1 \\ 0 & 1 & 0 \end{pmatrix}^{-1} = \begin{pmatrix} 1 & 1 & 2 \\ 0 & 0 & 1 \\ 0 & -1 & -2 \end{pmatrix}$, which gives $\langle\psi_1^l| = \begin{pmatrix} 1 & 1 & 2 \end{pmatrix}$, $\langle\tilde{h}_1^l| = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix}$, and $\langle\tilde{h}_2^l| = \begin{pmatrix} 0 & -1 & -2 \end{pmatrix}$. Finally, we find (see Supplementary Note 4):

$$\begin{aligned} G_{\text{new}}(\omega) &= \frac{|\psi_1^r\rangle\langle\psi_1^l|}{\omega - 1} + \frac{|h_1^r\rangle\langle\tilde{h}_1^l|}{\omega - 2} + \frac{|h_1^r\rangle\langle\tilde{h}_2^l|}{(\omega - 2)^2} + \frac{|h_2^r\rangle\langle\tilde{h}_2^l|}{\omega - 2} \\ &= \begin{pmatrix} \frac{1}{\omega-1} & \frac{1}{\omega-1} - \frac{1}{\omega-2} & \frac{2}{\omega-1} - \frac{2}{\omega-2} \\ 0 & \frac{2}{(\omega-2)^2} + \frac{1}{\omega-2} & \frac{4}{(\omega-2)^2} \\ 0 & -\frac{1}{(\omega-2)^2} & \frac{1}{\omega-2} - \frac{2}{(\omega-2)^2} \end{pmatrix}. \end{aligned} \tag{14}$$

One can easily verify that $G(\omega) = TG_{\text{new}}T^{-1}$ (see Supplementary Note 4). Importantly, we note that the matrix form here is not as simple as before. This is because the eigenvectors and the canonical vectors in this representation do not coincide with the canonical basis $\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$, which in turn gives rise to a more complicated matrix form with some elements featuring an interference between Lorentzian and square Lorentzian responses (the terms proportional to $\frac{1}{\omega - x}$ and $\frac{1}{(\omega-x)^2}$, respectively, for any number x). Evidently, the simple method presented here for calculating the left basis, which is one of the main results of this work, facilitates the evaluation of the linear response.

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3. Discussion and conclusion

We have presented a transparent derivation for the resolvent operator expansion in terms of the eigenvectors and canonical vectors associated with discrete non-Hermitian Hamiltonians. In contrast to our previous work [9], our derivation here highlights the connection with the structure of the underlying eigenspace decomposition. Finally, we have also presented a simple solution to the problem of self-orthogonality that arises when dealing with the left and right Jordan canonical vectors and shown how the left basis can be constructed in a systematic fashion using a single matrix inversion process.

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Supplemental document. See Supplement 1 for supporting content.

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