SPECTRA OF $\mathcal{PT}$-SYMMETRIC OPERATORS UNDER RANK-ONE PERTURBATIONS

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Abstract. We study the spectra of $\mathcal{PT}$-symmetric Hamiltonians H that are rank-one perturbations of a self-adjoint $\mathcal{PT}$-symmetric Hamiltonian H_0. We show that the discrete spectrum of H may include any number of complex-conjugate pairs of complex numbers of arbitrary algebraic multiplicity

1. Introduction

In their seminal paper [7], C. Bender and S. Boettcher studied a family of (generally non-Hermitian) Hamiltonians

$$-\frac{d^2}{dx^2} - (ix)^\alpha$$

and showed that, when $\alpha \geq 2$, they have only real eigenvalues. The authors suggested that such a rather unusual phenomenon was due to the fact that the non-real potential $V(x) := -(ix)^\alpha$ possesses the so-called $\mathcal{PT}$-symmetry property, in the sense that $\mathcal{PT}V(x) = V(x)\mathcal{PT}$. Here $\mathcal{P}$ and $\mathcal{T}$ are the *space parity* and *time reversal* operators respectively, defined as $(\mathcal{P}f)(x) = f(-x)$ and $(\mathcal{T}f)(x) = \overline{f(x)}$. That paper initiated a new branch of quantum mechanics called $\mathcal{PT}$-symmetric quantum mechanics [8–10] that has found numerous experimental confirmations [5]. Soon afterwards, dozens of non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians with real spectra were discovered, as well as many $\mathcal{PT}$-symmetric Hamiltonians possessing non-real eigenvalues; see [5] for an extensive review of the related physical bibliography and the book [6] for a wide overview of the current state of the art of the field.

Much work has been done since then to find sufficient and/or necessary conditions for reality of the spectrum of $\mathcal{PT}$-symmetric Hamiltonians. In particular, reality of the spectrum was understood to depend on the *exact*, or *unbroken* $\mathcal{PT}$-symmetry [11,17], for Hamiltonians with

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a hidden symmetry—i.e., a metric, or *charge conjugation operator* [4], for quasi-Hermitian [21] or pseudo-Hermitian Hamiltonians [29–31] etc.

Some results were obtained by developing perturbation theory for $\mathcal{PT}$-symmetric Hamiltonians [12–15]. Assume that H_0 is a $\mathcal{PT}$-symmetric Hamiltonian with discrete spectrum, H_0' is its relatively bounded $\mathcal{PT}$-symmetric perturbation, and $H_\varepsilon := H_0 + \varepsilon H_0'$. As the discrete spectrum of every $\mathcal{PT}$-symmetric Hamiltonian is symmetric with respect to the real line, every real simple eigenvalue must remains simple and thus real for small ε. On the contrary, non-simple eigenvalues (i.e., eigenvalues of multiplicity larger than one) often split and move into complex domain when ε departs from zero.

The purpose of this paper is to discuss spectra of H_0 under $\mathcal{PT}$-symmetric additive perturbations that are "small" in a different sense, namely, are of rank one. In the finite-dimensional setting, spectra of matrices under rank-one perturbations were shown in [22] to change quite arbitrarily; that result was also specified for structured (normal, Hermitian and unitary) matrices. The approach of [22] is purely algebraic and is based on the perturbation analysis of the related determinants; for that reason, it allows no direct generalization to infinite-dimensional setting. Behaviour of the Jordan structure of a matrix or operator under a generic rank-one or low-rank perturbations was discussed in [16, 19, 34, 35], while perturbation of structured matrices (such as real, symmetric, symplectic, orthogonal in Euclidean or indefinite inner product spaces) and matrix pencils have recently been discussed in [2,3,18,23–28,33]. A detailed spectral analysis of rank-one perturbations of self-adjoint Hamiltonians was made in [36].

In this paper, we prove that a rank-one $\mathcal{PT}$-symmetric perturbation of a self-adjoint Hamiltonian can dramatically change its discrete spectrum. Namely, we shall demonstrate that, using such perturbations, the discrete spectrum of any Hermitian $\mathcal{PT}$-symmetric Hamiltonian operator can be changed at will to contain any desired finite set of complex conjugate pairs of bound states with any desired degeneracy. More explicitly, we prove that, given an arbitrary self-adjoint and $\mathcal{PT}$-symmetric Hamiltonian H_0 with discrete spectrum, for any number n of non-real complex-conjugate pairs $z_1, \overline{z_1},\ z_2, \overline{z_2}, \dots, z_n, \overline{z_n}$, and any sequence of natural numbers $m_1, m_2, \dots, m_n$ there is a $\mathcal{PT}$-symmetric rank-one perturbation H of H_0 such that z_k and $\overline{z_k}$ are eigenvalues of H of (algebraic) multiplicity m_k for every $k = 1, 2, \dots, n$. In addition, our proof leads to an algorithm of constructing rank-one perturbations of desired spectral effect. These facts demonstrate that reality of the spectra of $\mathcal{PT}$-symmetric Hamiltonians is a non-trivial phenomenon, whose understanding requires deep mathematical analysis.

The paper is organized as follows. In the next section, we discuss general properties of $\mathcal{PT}$-symmetric Hamiltonians and their rank-one perturbations. In Section 3, we give an example of a rank-one $\mathcal{PT}$-symmetric perturbation of the kinetic Hamiltonian having eigenvalues at the points $\pm i$ and then prove a more general statement in Theorem 3.2 that any $2n$ eigenvalues of an arbitrary self-adjoint $\mathcal{PT}$-symmetric Hamiltonian H_0 can be moved into arbitrary n complex conjugate eigenvalue pairs by a $\mathcal{PT}$-symmetric rank-one perturbation. Then in Section 4, we demonstrate by example that a rank-one $\mathcal{PT}$-symmetric perturbation can lead to degenerate non-real eigenvalues and then prove in Theorem 4.2 that, for every self-adjoint $\mathcal{PT}$-symmetric Hamiltonian H_0 and any $2n$ of its eigenvalues, a $\mathcal{PT}$-symmetric rank-one perturbation H of H_0 exists for which the selected eigenvalues get transformed into an eigenvalue pair z and $\overline{z}$ of multiplicity n. We combine the above two effects into the most general Theorem 5.1 in Section 5 and explain how it applies to the quantum harmonic oscillator. Finally, Section 6 summarizes the results and discusses possible generalizations.

2. Preliminaries

Assume that $\mathcal{H}$ is a separable Hilbert space with inner product $\langle\cdot,\cdot\rangle$ (linear in the first component and anti-linear in the second one) and H_0 is a self-adjoint Hamiltonian in $\mathcal{H}$ with simple discrete spectrum. Under this assumption, the operator H_0 is necessarily unbounded, has compact resolvent, and its spectrum $\sigma(H_0)$ consists of real simple eigenvalues that can be listed in increasing order as λ_n, $n\in I$, where $I=\mathbb{N}$ if H_0 is bounded below and $I=\mathbb{Z}$ if it is bounded neither below nor above. We denote by v_n, $n\in I$, the corresponding normalized eigenfunctions.

Next we introduce the abstract notions of the *space parity* operator $\mathcal{P}$ and *time reversal* operator $\mathcal{T}$ in $\mathcal{H}$; these are modelled by bounded commuting operators in $\mathcal{H}$ with the following properties:

(a) $\mathcal{P}$ is a unitary involution, i.e., $\mathcal{P}^2=I$ and, for all f and g in $\mathcal{H}$,
$$\langle\mathcal{P}f,\mathcal{P}g\rangle=\langle f,g\rangle;$$

(b) $\mathcal{T}$ is a conjugation operator, i.e., $\mathcal{T}^2=I$ and for all f and g in $\mathcal{H}$
$$\langle\mathcal{T}f,\mathcal{T}g\rangle=\langle g,f\rangle.$$

Clearly, the operators $(\mathcal{P}f)(x)=f(-x)$ and $(\mathcal{T}f)(x)=\overline{f(x)}$ in the Hilbert space $\mathcal{H}=L_2(\mathbb{R})$ are just standard particular examples of such symmetries. A mirror symmetry with respect to any hyperplane in $\mathbb{R}^n$

through the origin is another example of the operator $\mathcal{P}$ in the Hilbert space $\mathcal{H} = L_2(\mathbb{R}^n)$.

Definition 2.1. A densely defined (unbounded) operator A is called $\mathcal{PT}$*-symmetric* if

$$\mathcal{PT}Af = A\mathcal{PT}f$$

for all f in the domain of A.

We assume that the unperturbed Hamiltonian H_0 is $\mathcal{PT}$-symmetric. This implies that $H_0(\mathcal{PT}v_n) = \mathcal{PT}(H_0v_n) = \lambda_n\mathcal{PT}v_n$, so that $\mathcal{PT}v_n$ is an eigenfunction of H_0 corresponding to the eigenvalue λ_n along with v_n. Since λ_n was assumed simple, we have $\mathcal{PT}v_n = c_nv_n$ for a complex c_n with $|c_n| = 1$. As observed in [9], by appropriate scaling this constant can be absorbed into v_n; then we have $\mathcal{PT}v_n = v_n$, i.e., there is no spontaneous symmetry breaking in H_0.

Our aim is to study spectral properties of the $\mathcal{PT}$-symmetric Hamiltonians H that are rank-one perturbations of H_0. We recall that a linear operator A acting in the infinite-dimensional space $\mathcal{H}$ is of rank one if the range $\operatorname{ran} A$ of A is one-dimensional. Taking an arbitrary non-zero vector $\psi \in \operatorname{ran} A$, we conclude that $Af = c(f)\psi$ for every $f \in \mathcal{H}$, with a bounded linear functional $c(f)$; as a result, there is $\varphi \in \mathcal{H}$ such that $Af = \langle f, \varphi\rangle\psi$. Therefore, a generic rank-one perturbation H of H_0 is of the form

$$H = H_0 + \langle \cdot, \varphi\rangle\psi, \tag{2.1}$$

where φ and ψ are fixed non-zero functions in $\mathcal{H}$, in the sense that

$$Hf = H_0f + \langle f, \varphi\rangle\psi$$

for every $f \in \operatorname{dom}(H) = \operatorname{dom}(H_0)$. Our primary objective is to understand how much the spectrum of H_0 can change under such rank-one perturbations.

We observe that the Hilbert space adjoint H^* of the rank-one perturbation H (2.1) of H_0 is given by

$$H^* = H_0 + \langle \cdot, \psi\rangle\varphi,$$

so that H is Hermitian (i.e., self-adjoint in the Hilbert space $\mathcal{H}$) if and only if the functions φ and ψ are collinear. $\mathcal{PT}$-symmetry of H requires quite different properties of φ and ψ, as the following lemma demonstrates.

Lemma 2.2. *The rank-one perturbation $\langle \cdot, \varphi\rangle\psi$ is $\mathcal{PT}$-symmetric if and only if there is a number $c \in \mathbb{C}$ with $|c| = 1$ such that $\mathcal{PT}\varphi = c\varphi$ and $\mathcal{PT}\psi = c\psi$.*

Proof. $\mathcal{PT}$-symmetry of the rank-one perturbation $A = \langle\cdot,\varphi\rangle\psi$ requires that, for every $f \in \mathcal{H}$,

$$\mathcal{PT}(Af) = \overline{\langle f,\varphi\rangle}\mathcal{PT}\psi = \langle\mathcal{PT}f,\varphi\rangle\psi = A(\mathcal{PT}f).$$

Therefore, $\mathcal{PT}\psi$ and ψ are collinear, i.e., $\mathcal{PT}\psi = c\psi$ for some complex number c; as $\mathcal{PT}$ is an isometry, we see that $|c| = 1$. The above relation now implies that $\langle\mathcal{PT}f,\varphi\rangle = c\langle\varphi,f\rangle$ for all $f \in \mathcal{H}$. Using properties of $\mathcal{P}$ and $\mathcal{T}$, we find that

$$\langle\mathcal{PT}f,\varphi\rangle = \langle\mathcal{T}f,\mathcal{P}\varphi\rangle = \langle\mathcal{PT}\varphi,f\rangle$$

and thus conclude that $\mathcal{PT}\varphi = c\varphi$ with the same constant c. □

Corollary 2.3. *Set $c = e^{i\alpha}$; replacing φ and ψ with $e^{i\alpha/2}\varphi$ and $e^{i\alpha/2}\psi$, respectively, we do not change the rank-one perturbation $\langle\cdot,\varphi\rangle\psi$ and reduce c to the case $c = 1$. Therefore, without loss of generality we can (and shall) assume that the functions φ and ψ are $\mathcal{PT}$-symmetric, i.e., that they satisfy the relations $\mathcal{PT}\varphi = \varphi$ and $\mathcal{PT}\psi = \psi$.*

Next we characterize the spectrum of the operator H; a useful instrument for that purpose is the *characteristic function* F of H defined for $\lambda \in \rho(H_0)$ via [1, Sec. 1.1.1]

$$F(\lambda) := \langle(H_0 - \lambda)^{-1}\varphi,\psi\rangle + 1. \tag{2.2}$$

Indeed, as explained in *loc. cit.*, if $\lambda \in \rho(H_0)$ is such that $F(\lambda) \neq 0$, then λ is in the resolvent set $\rho(H)$ of H and the resolvent $(H - \lambda)^{-1}$ satisfies the Krein resolvent formula

$$(H - \lambda)^{-1} = (H_0 - \lambda)^{-1} - \frac{\langle\,\cdot\,,(H_0 - \overline{\lambda})^{-1}\varphi\rangle}{F(\lambda)}\,(H_0 - \lambda)^{-1}\psi.$$

Therefore, the resolvent $(H - \lambda)^{-1}$ is compact whence H has a discrete spectrum.

Denote by a_n and b_n the Fourier coefficients of the vectors φ and ψ with respect to the orthonormal basis of eigenfunctions v_n,

$$\varphi = \sum_{n\in I} a_n v_n, \qquad \psi = \sum_{n\in I} b_n v_n. \tag{2.3}$$

Set

$$I_0 := \{n \in I \mid a_n b_n = 0\}, \qquad I_1 := \{n \in I \mid a_n b_n \neq 0\};$$

it was shown in [16] that the intersection $\sigma(H_0) \cap \sigma(H) =: \sigma_0(H)$ coincides with the set $\{\lambda_n \mid n \in I_0\}$. Next, using the spectral theorem for the Hamiltonian H_0, we can write the characteristic function F of H in (2.2) as

$$F(\lambda) = \sum_{n\in I_1} \frac{\overline{a_n}b_n}{\lambda_n - \lambda} + 1; \tag{2.4}$$

then another interesting result proved in [16] is the following relation between the zeros of F and the bound states of H.

Proposition 2.4. *Zeros of F coincide with the bound states of H including multiplicities, i.e., if λ is a zero of F of multiplicity $k \geq 1$, then λ is a bound state of H of algebraic multiplicity k if $\lambda \notin \sigma_0(H)$ and of algebraic multiplicity $k+1$ otherwise.*

We recall that algebraic and geometric multiplicity of an eigenvalue are defined as follows [20]. Assume that λ is an isolated point of the spectrum $\sigma(A)$ of a linear operator A. We form the corresponding Riesz spectral projector

$$P_\lambda = \frac{1}{2\pi i} \int_\Gamma (A - z)^{-1}\, dz, \tag{2.5}$$

where Γ is a contour in the resolvent set of A whose interior contains λ but no other points of $\sigma(A)$, and call the dimension $\dim \operatorname{ran} P_\lambda$ of the range of P_λ the *algebraic multiplicity* of the eigenvalue λ. If the algebraic multiplicity of λ is finite, then it coincides with the dimension of the root subspace, i.e., the set of all vectors v for which there is $k \in \mathbb{N}$ such that $(A - \lambda)^k v = 0$. The *geometric multiplicity* of the eigenvalue λ is the dimension of the nullspace of the operator $A - \lambda$. An eigenvalue λ is called semi-simple if its algebraic multiplicity coincides with the geometric one.

Proposition 2.4 gives an effective tool of constructing a rank-one perturbation H with the prescribed set of non-real degenerate bound states through constructing the characteristic function (2.4) with prescribed zeros of desired multiplicities. Following this path, it was shown in [16] that, under no $\mathcal{PT}$-symmetry assumptions, the perturbed Hamiltonian H can possess an arbitrary non-real spectrum of arbitrary algebraic multiplicity. However, $\mathcal{PT}$-symmetry of H imposes some restrictions on its bound states and their multiplicities, as well as on the functions φ and ψ.

Firstly, although a $\mathcal{PT}$-symmetric Hamiltonian H may have non-real eigenvalues, they necessarily come in complex conjugate pairs: indeed, if λ is an eigenvalue of H with eigenvector v, then the equality $H(\mathcal{PT}v) = \overline{\lambda}\mathcal{PT}v$ shows that $\overline{\lambda}$ is also an eigenvalue of H with eigenvector $\mathcal{PT}v$. Secondly, it follows from the formula (2.5) for the Riesz projector that the root subspaces $\mathcal{H}_\lambda$ and $\mathcal{H}_{\overline{\lambda}}$ of H for the eigenvalues λ and $\overline{\lambda}$ satisfy the relation $\mathcal{H}_{\overline{\lambda}} = \mathcal{PT}\mathcal{H}_\lambda$, which shows that the algebraic multiplicities of λ and $\overline{\lambda}$ coincide. Finally, $\mathcal{PT}$-symmetry of φ and v_n

implies that

$$\sum_{n\in I} a_n v_n = \varphi = \mathcal{PT}\varphi = \sum_{n\in I} \overline{a_n} v_n,$$

so that the Fourier coefficients a_n of φ are real; in the same manner we show that all Fourier coefficients b_n of ψ are real.

It follows from [16] that the eigenvalues of H can be labelled by μ_n, $n \in I$, in such a way that each μ_n is repeated according to its algebraic multiplicity and $|\mu_n - \lambda_n| \to 0$ as $|n| \to \infty$. As a result, the eigenvalues μ_n of H with sufficiently large $|n|$ are simple and real, so that H may have at most finitely many non-real eigenvalues. We shall prove in the following sections that except for these restriction (of finiteness and symmetry including multiplicities), the non-real spectrum of H can be arbitrary.

3. Non-real eigenvalues

We start with the following example that will serve as a motivation for the more general results.

Example 3.1. Let $\mathcal{H}$ be the Hilbert space $L_2(-\pi, \pi)$, with the standard space parity $\mathcal{P}f(x) = f(-x)$ and time reversal $\mathcal{T}f(x) = \overline{f(x)}$. We consider in $\mathcal{H}$ a kinetic Hermitian Hamiltonian $H_0 = -\frac{d^2}{dx^2}$ subject to the Neumann boundary conditions $y'(-\pi) = y'(\pi) = 0$. The spectrum of H_0 coincides with $\lambda_n := n^2$ for $n \in \mathbb{Z}_+$, and the normalized eigenfunction for the eigenvalue λ_n is the constant $v_0(x) = 1/\sqrt{2\pi}$ if $n = 0$ and $v_n(x) := \cos nx/\sqrt{\pi}$ if $n > 0$.

We will construct a rank one perturbation $H = H_0 + \langle\,\cdot\,, \varphi\rangle\psi$ of H_0 which is $\mathcal{PT}$-symmetric and shares with H_0 all its eigenvalues except λ_0 and λ_1, these being moved to $\pm i$. According to [16], φ and ψ can be taken to be linear combinations of v_0 and v_1, i.e.,

$$\varphi(x) = a_0 v_0 + a_1 v_1, \qquad \psi(x) = b_0 v_0 + b_1 v_1.$$

As we mentioned in Section 2, the rank-one perturbation H is $\mathcal{PT}$-symmetric if $\mathcal{PT}\varphi = \varphi$ and $\mathcal{PT}\psi = \psi$; with the above form of φ and ψ, this is equivalent to having a_0, a_1, b_0, and b_1 real.

The characteristic function F of H in (2.4) reads

$$F(z) = \frac{\overline{a_0} b_0}{-z} + \frac{\overline{a_1} b_1}{1 - z} + 1,$$

and we need to satisfy two equations,

$$F(i) = F(-i) = 0.$$

This leads to a linear system of two equations in variables $x = \overline{a_0} b_0$ and $y = \overline{a_1} b_1$ possessing the unique solution, $x = 1$ and $y = -2$. One

of the many choices for the Fourier coefficients can be $a_0 = b_0 = 1$, $a_1 = -b_1 = \sqrt{2}$, leading to

$$\varphi(x) = \frac{1 + 2\cos x}{\sqrt{2\pi}}, \qquad \psi(x) = \frac{1 - 2\cos x}{\sqrt{2\pi}}.$$

Therefore, the corresponding operator H is

$$H = -\frac{d^2}{dx^2} + \frac{1}{2\pi}\langle\,\cdot\,, 1 + 2\cos x\rangle(1 - 2\cos x)$$

with $\mathrm{dom}(H) = \mathrm{dom}(H_0)$. By construction, $v_k \perp \varphi$ for $k > 1$, so that each such v_k is an eigenfunction of H corresponding to the eigenvalue $\mu_k = k^2$. A direct verification shows that $w_\pm := 1 \pm i - 2\cos x$ satisfy the relations $Hw_\pm = \pm i w_\pm$ and thus are the eigenfunctions for the eigenvalues $\pm i$. As the set of functions $\{v_k\}_{k>1} \cup \{w_\pm\}$ is a basis of $\mathcal{H}$, we conclude that H has no other eigenvalues, so that the set $\{k^2\}_{k>1} \cup \{\pm i\}$ is the spectrum of H as claimed.

More generally, the next theorem shows that any $2n$ real eigenvalues of H_0 can be moved to any n pairs of (non-real) complex conjugate points by a $\mathcal{PT}$-symmetric rank one perturbation.

Theorem 3.2. *Assume that H_0 is a self-adjoint operator in a Hilbert space $\mathcal{H}$ that is also $\mathcal{PT}$-symmetric with respect to certain space parity $\mathcal{P}$ and time reversal $\mathcal{T}$. Assume further that H_0 has a compact resolvent and denote by $\sigma(H_0) := \{\lambda_k\}_{k\in I}$ the spectrum of H_0. Then for every $n \in \mathbb{N}$, every n pairwise distinct points $z_1, z_2, \ldots, z_n$ in the upper complex half-plane $\mathbb{C}_+$, and every set of $2n$ pairwise distinct eigenvalues $\lambda_{k_1}, \lambda_{k_2}, \ldots, \lambda_{k_{2n}}$ of H_0 there exists a rank-one $\mathcal{PT}$-symmetric perturbation H of H_0 whose spectrum is*

$$\big(\sigma(H_0) \setminus \{\lambda_{k_j}\}_{j=1}^{2n}\big) \cup \{z_1, \overline{z_1}, z_2, \overline{z_2}, \ldots, z_n, \overline{z_n}\}.$$

Proof. For convenience, we denote by $\mu_j := \lambda_{k_j}$ and $w_j := v_{k_j}$, $j = 1, \ldots, 2n$, the chosen eigenvalues and the corresponding eigenvectors of the operator H_0. Also, set $\omega_k := z_k$ and $\omega_{k+n} := \overline{z_k}$ for $k = 1, 2, \ldots, n$. It follows from the considerations of Section 2 that the functions φ and ψ in the rank-one perturbation H of H_0 can be chosen from the subspace $\mathcal{H}_0 := \mathrm{ls}\{w_1, w_2, \ldots, w_{2n}\}$, so that

$$\varphi = \sum_{j=1}^{2n} c_j w_j, \qquad \psi = \sum_{j=1}^{2n} d_j w_j \tag{3.1}$$

for some c_j and d_j. We set $x_j := \overline{c_j} d_j$ for $j = 1, \dots, 2n$; then the characteristic function of $H = H_0 + \langle \cdot\,, \varphi \rangle \psi$ is equal to

$$F(z) := \sum_{j=1}^{2n} \frac{x_j}{\mu_j - z} + 1,$$

and we look for x_j such that F has $2n$ zeros $\omega_1, \omega_2, \dots, \omega_{2n}$. The equalities

$$F(\omega_1) = F(\omega_2) = \cdots = F(\omega_{2n}) = 0$$

form a linear inhomogeneous system of $2n$ equations for $2n$ variables $x_1, x_2, \dots, x_{2n}$, viz.

$$\frac{x_1}{\mu_1 - \omega_k} + \frac{x_2}{\mu_2 - \omega_k} + \cdots + \frac{x_{2n}}{\mu_{2n} - \omega_k} = -1, \qquad k = 1, 2, \dots, 2n. \tag{3.2}$$

The coefficient matrix M of that system has entries

$$m_{kj} := \frac{1}{\mu_j - \omega_k}$$

and thus is a non-singular Cauchy matrix [32].

It follows that system (3.2) has a unique solution $x_1, x_2, \dots, x_{2n}$. Taking now conjugates of each equation in (3.2), we arrive at the system

$$\sum_{j=1}^{2n} \frac{\overline{x_j}}{\mu_j - \overline{\omega_k}} + 1 = 0, \qquad k = 1, 2, \dots, 2n.$$

Since $\overline{\omega_k} = \omega_{k+n}$ for $k = 1, 2, \dots, n$, we see that $\overline{x_1}, \overline{x_2}, \dots, \overline{x_{2n}}$ is also a solution of the linear system (3.2). By uniqueness of solutions, we conclude that every x_j satisfies $x_j = \overline{x_j}$ and thus is real.

The functions φ and ψ can be formed e.g. by taking $c_1 = c_2 = \cdots = c_{2n} = 1$ and $d_j = x_j$, $j = 1, 2, \dots, 2n$, in formula (3.1). With such a choice, the rank-one perturbation H of the operator H_0 will be $\mathcal{PT}$-symmetric. By construction, H coincides with H_0 on the orthogonal complement of $\mathcal{H}_0$; therefore, every eigenvalue λ_k of H_0 not in the set $\mu_1, \mu_2, \dots, \mu_{2n}$ is also an eigenvalue of H with the same eigenvector v_k. By [1, 16], H also possess eigenvalues at the points $\omega_1, \omega_2, \dots, \omega_{2n}$. As the eigenvectors of H corresponding to those eigenvalues form a basis of $\mathcal{H}_0$, we conclude that H has a complete set of eigenfunctions in $\mathcal{H}$ and thus possesses no other eigenvalues. The proof is complete. □

4. Non-simple eigenvalues

Self-adjoint operators in a Hilbert space have (semi-)simple eigenvalues in the sense that the corresponding root subspaces coincide with

the eigenspaces, i.e., that every non-zero root vector is an eigenvector. For a non-self-adjoint operator H, however, there may exists the so-called Jordan chains of eigen- and associated vectors $w_0, w_1, \dots, w_n$ for an eigenvalue λ, so that $Hw_0 = \lambda w_0$ and $Hw_j = \lambda w_j + w_{j-1}$ for $j = 1, 2, \dots, n$. We start with an example of a rank-one $\mathcal{PT}$-symmetric perturbation H of a self-adjoint operator H_0 such that H has non-semi-simple non-real eigenvalues.

Example 4.1. We take the same Hilbert space $\mathcal{H} = L_2(-\pi, \pi)$ and the $\mathcal{P}$ and $\mathcal{T}$ symmetries as in Example 3.1. Consider the self-adjoint $\mathcal{PT}$-symmetric momentum operator $H_0 = \frac{1}{i}\frac{d}{dx}$ with periodic boundary conditions; its spectrum coincides with the set $\mathbb{Z}$, and a normalized eigenfunction v_n corresponding to the eigenvalue $\lambda_n := n$ is equal to $e^{inx}/\sqrt{2\pi}$.

We shall construct a $\mathcal{PT}$-symmetric rank-one perturbation H (2.1) whose spectrum consists of simple eigenvalues $k \in \mathbb{Z} \setminus \{\pm 1, \pm 2\}$ and eigenvalues $\pm i$ each of algebraic multiplicity 2 (i.e., generating Jordan chains of eigen- and associated vectors of length 2).

According to the results of [16], the functions φ and ψ can be taken as linear combinations of the vectors v_{-2}, v_{-1}, v_1 and v_2, so that

$$\varphi = a_{-2}v_{-2} + a_{-1}v_{-1} + a_1 v_1 + a_2 v_2, \qquad \psi = b_{-2}v_{-2} + b_{-1}v_{-1} + b_1 v_1 + b_2 v_2.$$

The characteristic function

$$F(z) = \frac{x_{-2}}{-2 - z} + \frac{x_{-1}}{-1 - z} + \frac{x_1}{1 - z} + \frac{x_2}{2 - z} + 1,$$

where $x_k = \overline{a_k} b_k$ for $k = \pm 1, \pm 2$, must obey the following relations:

$$F(i) = F'(i) = F(-i) = F'(-i) = 0.$$

The equations $F'(\pm i) = 0$ read

$$\frac{x_{-2}}{(2 \pm i)^2} + \frac{x_{-1}}{(1 \pm i)^2} + \frac{x_1}{(1 \mp i)^2} + \frac{x_2}{(2 \mp i)^2} = 0;$$

adding them, we conclude that $x_{-2} + x_2 = 0$, and subtracting now the equation $F(i) = 0$ from $F(-i) = 0$ results in the relation $x_{-1} + x_1 = 0$. Therefore, we obtain the following system of two equations in x_1 and x_2:

$$\begin{aligned} \frac{4}{5}x_2 + x_1 &= -1, \\ \frac{8}{25}x_2 + x_1 &= 0, \end{aligned}$$

with unique solution $x_2 = -25/12 = -x_{-2}$ and $x_1 = 2/3 = -x_{-1}$.

Now we can choose, e.g., the rank-one perturbation corresponding to $a_{-2} = a_{-1} = a_1 = a_2 = 1$ and $b_j = x_j$ for $j = -2, -1, 1$, and 2. As the

coefficients a_j and b_j are real, we conclude that the corresponding rank-one perturbation H of the self-adjoint operator H_0 is $\mathcal{PT}$-symmetric.

To show that the constructed operator H possesses eigenvalues $\pm i$, both of algebraic multiplicity 2, we note that the 4-dimensional subspace $\mathcal{H}_0 := \mathrm{ls}\{e^{-2ix}, e^{-ix}, e^{ix}, e^{2ix}\}$ is invariant under H. The corresponding matrix representation of the restriction of H onto $\mathcal{H}_0$ is a matrix of size 4, whose eigenvalues are precisely $\pm i$, both of multiplicity 2. Eigenfunction completeness guarantee that H has no other eigenvalues except $\pm i$ and the common eigenvalues $\mathbb{Z} \setminus \{-2, -1, 1, 2\}$.

We can now generalize the above example as follows.

Theorem 4.2. *Assume that H_0 is a self-adjoint Hamiltonian in a Hilbert space $\mathcal{H}$ that is also $\mathcal{PT}$-symmetric with respect to certain space parity $\mathcal{P}$ and time reversal $\mathcal{T}$. Assume further that H_0 has a compact resolvent and denote by $\sigma(H_0) := \{\lambda_k\}_{k\in I}$ the spectrum of H_0. Then for every $n \in \mathbb{N}$, every non-real z_0 in the upper complex half-plane $\mathbb{C}_+$, and every set of $2n$ pairwise distinct eigenvalues $\lambda_{k_1}, \lambda_{k_2}, \ldots, \lambda_{k_{2n}}$ of H_0 there exists a rank-one $\mathcal{PT}$-symmetric perturbation H of H_0 whose spectrum is*

$$\big(\sigma(H_0) \setminus \{\lambda_{k_j}\}_{j=1}^{2n}\big) \cup \{z_0, \overline{z_0}\},$$

and the eigenvalues z_0 and $\overline{z_0}$ are of algebraic multiplicity n and possess chains of eigen- and associated vectors of length n.

Proof. The proof is constructive and similar to that of Theorem 3.2. For convenience, we denote by $\mu_j := \lambda_{k_j}$ and $w_j := v_{k_j}$, $j = 1, \ldots, 2n$, the chosen eigenvalues and the corresponding eigenvectors of the operator H_0. It follows from the considerations of Section 2 that the functions φ and ψ in the rank-one perturbation H of H_0 can be searched for in the subspace $\mathcal{H}_0 := \mathrm{ls}\{w_1, w_2, \ldots, w_{2n}\}$, so that

$$\varphi = \sum_{j=1}^{2n} c_j w_j, \qquad \psi = \sum_{j=1}^{2n} d_j w_j \tag{4.1}$$

for some c_j and d_j. We set $x_j := \overline{c_j} d_j$ for $j = 1, \ldots, 2n$; then the characteristic function of $H = H_0 + \langle \cdot\,, \varphi\rangle\psi$ is equal to

$$F(z) := \sum_{j=1}^{2n} \frac{x_j}{\mu_j - z} + 1,$$

and we look for x_j such that F has zeros z_0 and $\overline{z_0}$, each of multiplicity n. The equalities

$$F(z_0) = F'(z_0) = \cdots = F^{(n-1)}(z_0) \\ = F(\overline{z_0}) = F'(\overline{z_0}) = \cdots = F^{(n-1)}(\overline{z_0}) = 0$$

form a linear inhomogeneous system of $2n$ equations for $2n$ variables $x_1, x_2, \ldots, x_{2n}$, viz.

$$\begin{array}{lll} \dfrac{x_1}{\mu_1 - z_0} + \ldots + \dfrac{x_{2n}}{\mu_{2n} - z_0} = -1, & & \\ \dfrac{x_1}{(\mu_1 - z_0)^k} + \ldots + \dfrac{x_{2n}}{(\mu_{2n} - z_0)^k} = 0, & k = 2, \ldots, n, \\ \dfrac{x_1}{\mu_1 - \overline{z_0}} + \ldots + \dfrac{x_{2n}}{\mu_{2n} - \overline{z_0}} = -1, & & \\ \dfrac{x_1}{(\mu_1 - \overline{z_0})^k} + \ldots + \dfrac{x_{2n}}{(\mu_{2n} - \overline{z_0})^k} = 0, & k = 2, \ldots, n. \end{array} \tag{4.2}$$

We prove in Lemma 4.3 below that the coefficient matrix of that system is non-singular. As a result, there is a unique solution $x_1, x_2, \ldots, x_{2n}$. By taking the complex conjugate of every equation in the above system, we get a solution $\overline{x_1}, \overline{x_2}, \ldots, \overline{x_{2n}}$ of the system with z_0 and $\overline{z_0}$ interchanged. As this merely amount to interchanging first n and the last n equations, we conclude that $\overline{x_1}, \overline{x_2}, \ldots, \overline{x_{2n}}$ is also a solution of the original system, so that $\overline{x_k} = x_k$ for each $k = 1, 2, \ldots, 2n$.

As a result, the numbers x_k are real, and we can take $c_k = 1$ and $d_k = x_k$ for $k = 1, 2, \ldots, 2n$ in formula (4.1). The resulting functions φ and ψ lead to a $\mathcal{PT}$-symmetric rank-one perturbation H of H_0 of (2.1). As the characteristic function (2.4) of that operator satisfies the above system, in view of [16] it has the required eigenvalues of prescribed multiplicities. Lack of other eigenvalues follows from completeness of eigenfunctions, and the proof is complete. □

Now we prove the fact that the coefficient matrix of the system (4.2) is non-singular. We fix pairwise distinct numbers $\mu_1, \mu_2, \ldots, \mu_{2n}$ and denote by $D(z_1, z_2, \ldots, z_{2n})$ the Cauchy determinant of the matrix M with entries

$$m_{jk} = \frac{1}{\mu_k - z_j}, \qquad j, k = 1, 2, \ldots, 2n.$$

It is known [32] that

$$D(z_1, z_2, \ldots, z_{2n}) = \frac{\prod \prod_{j>k} (\mu_j - \mu_k)(z_j - z_k)}{\prod_j \prod_k (\mu_j - z_k)}. \tag{4.3}$$

Lemma 4.3. *The coefficient matrix of system* (4.2) *is non-singular.*

Proof. We use row linearity of determinants to derive the explicit formula for the determinant of the coefficient matrix in (4.2). On the first step, we replace rows 2 to n of the matrix $M = M_1$ by their differences with the first row to obtain the matrix M_1'. The j^{th} row of M_1', $j = 2, \dots, n$, has entries

$$\frac{z_j - z_1}{(\mu_k - z_1)(\mu_k - z_j)}, \qquad k = 1, 2, \dots, 2n.$$

As the determinant of the resulting matrix does not change under such a transformation, we see that

$$D(z_1, z_2, \dots, z_{2n}) = D_2(z_1, z_2, \dots, z_{2n}) \prod_{j=2}^{n} (z_j - z_1),$$

where $D_2(z_1, z_2, \dots, z_{2n})$ is the determinant of the $(2n) \times (2n)$ matrix M_2, whose rows $j = 2$ to $j = n$ have entries

$$\frac{1}{(\mu_k - z_1)(\mu_k - z_j)}, \qquad k = 1, 2, \dots, 2n,$$

and the rest rows are the same as in the matrix M_1.

On the second step, we subtract the second row of the matrix M_2 from its rows $j = 3$ to $j = n$; the resulting j^{th} row then becomes

$$\frac{z_j - z_2}{(\mu_k - z_1)(\mu_k - z_2)(\mu_k - z_j)}, \qquad k = 1, 2, \dots, 2n.$$

Therefore,

$$D_2(z_1, z_2, \dots, z_{2n}) = D_3(z_1, z_2, \dots, z_{2n}) \prod_{j=3}^{n} (z_j - z_2),$$

where $D_3(z_1, z_2, \dots, z_{2n})$ is the determinant of the matrix M_3, which is M_2 with rows $j = 3$ to $j = n$ replaced by the ones with entries

$$\frac{1}{(\mu_k - z_1)(\mu_k - z_2)(\mu_k - z_j)}, \qquad k = 1, 2, \dots, 2n.$$

Continuing this process, we get a sequence of matrices M_m and their determinants $D_m(z_1, z_2, \dots, z_{2n})$, $m = 2, 3, \dots, n$, defined recursively via

$$D_{m-1}(z_1, z_2, \dots, z_{2n}) = D_m(z_1, z_2, \dots, z_{2n}) \prod_{j=m}^{n} (z_j - z_m). \tag{4.4}$$

In particular, D_n is the determinant of the matrix M_n whose j^{th} row, $j = 1, 2, \dots, n$, has entries

$$(\mu_k - z_1)^{-1} \cdots (\mu_k - z_j)^{-1}, \qquad k = 1, 2, \dots, 2n,$$

and rows $n+1$ to $2n$ are the same as in the matrix M_1.

We now repeat the above process for rows $n+1$ to $2n$ of the matrix $M_{n+1} := M_n$: first, we subtract the $(n+1)^{\text{st}}$ row from the rows $n+2$ to $2n$, then the row $n+2$ from rows $n+3$ to $2n$ of the resulting matrix, and so on. After this procedure, we obtain the matrix M_{2n}, whose j^{th} row, $j = n+1, \dots, 2n$, has entries

$$(\mu_k - z_{n+1})^{-1}(\mu_k - z_{n+2})^{-1} \cdots (\mu_k - z_{n+j})^{-1}, \qquad k = 1, 2, \dots, 2n.$$

The determinant of M_{2n} can be found explicitly using (4.3) and the recursive relations between D_{m-1} and D_m; as a result, we find that

$$D_{2n}(z_1, z_2, \dots, z_{2n}) = \frac{\prod_{j>k}(\mu_j - \mu_k) \prod_{j=n+1}^{2n} \prod_{k=1}^{n} (z_j - z_k)}{\prod_j \prod_k (\mu_j - z_k)}.$$

It remains to observe that the coefficient matrix of interest is the M_{2n} with $z_1 = z_2 = \cdots = z_n = z_0$ and $z_{n+1} = z_{n+2} = \cdots = z_{2n} = \overline{z_0}$; therefore, its determinant is equal to

$$D_{2n}(z_0, z_0, \dots, z_0, \overline{z_0}, \overline{z_0}, \dots, \overline{z_0}) = \frac{(\overline{z_0} - z_0)^{n^2} \prod_{j>k}(\mu_j - \mu_k)}{\prod_{j=1}^{2n} |\mu_j - z_0|^{2n}}.$$

As that determinant is non-zero for $z_0 \in \mathbb{C}_+$, the proof is complete. $\square$

5. Possible non-real spectrum of H

We now combine the approaches of Sections 3 and 4 to prove the general result of this paper on non-real spectra of $\mathcal{PT}$-symmetric rank-one perturbations H of H_0. Take an arbitrary n, then an n-tuple $(m_1, \dots, m_n)$ of natural numbers, and a set $M := \{z_1, \dots, z_n\} \subset \mathbb{C}_+$ of n pairwise distinct non-real numbers from the upper complex half-plane. Set $N := 2(m_1 + m_2 + \cdots + m_n)$, choose any N pairwise distinct eigenvalues $\lambda_{k_1}, \lambda_{k_2}, \dots, \lambda_{k_N}$ of H_0, and set $\Lambda_0 := \sigma(H_0) \setminus \{\lambda_{k_1}, \lambda_{k_2}, \dots, \lambda_{k_N}\}$.

Theorem 5.1. *Under the above assumptions, there is a $\mathcal{PT}$-symmetric rank-one perturbation H of H_0 whose spectrum is*

$$\sigma(H) = \Lambda_0 \cup M \cup \overline{M}$$

and the eigenvalues z_k and $\overline{z_k}$, $k = 1, \dots, n$, are of multiplicity m_k.

Proof. The proof is derived by combining the main steps of the proofs of Theorems 3.2 and 4.2. For convenience, we denote by $\mu_j := \lambda_{k_j}$ and $w_j := v_{k_j}$, $j = 1, \dots, N$, the chosen eigenvalues and the corresponding

eigenvectors of the operator H_0. The functions φ and ψ in the rank-one perturbation H of H_0 can be searched for in the subspace $\mathcal{H}_0 := \mathrm{ls}\{w_1, w_2, \dots, w_N\}$, so that

$$\varphi = \sum_{j=1}^{N} c_j w_j, \qquad \psi = \sum_{j=1}^{N} d_j w_j \tag{5.1}$$

for some c_j and d_j. We set $x_j := \overline{c_j} d_j$ for $j = 1, \dots, N$; then the characteristic function of $H = H_0 + \langle \cdot\,, \varphi\rangle\psi$ is equal to

$$F(z) := \sum_{j=1}^{N} \frac{x_j}{\mu_j - z} + 1,$$

and we look for x_j such that F has zeros of multiplicity m_k at the points z_k and $\overline{z_k}$ for $k = 1, \dots, n$. The equalities

$$\begin{aligned} F(z_k) = F'(z_k) = \cdots = F^{(m_k-1)}(z_k) \\ = F(\overline{z_k}) = F'(\overline{z_k}) = \cdots = F^{(m_k-1)}(\overline{z_k}) = 0 \end{aligned} \tag{5.2}$$

for $k = 1, 2, \dots, n$ give an inhomogeneous system of size N in variables $x_1, x_2 \dots, x_N$ whose coefficient matrix M has rows of entries

$$\frac{1}{(\mu_j - \omega_k)^m}, \qquad k = 1, \dots, n, \quad m = 1, \dots, m_k,$$

where $\omega_k = z_k$ and $\omega_k = \overline{z_k}$ in the top and the bottom halves of the matrix M, respectively.

Small amendments in the proof of Lemma 4.3 (where z_0 is consecutively replaced with $z_1, z_2, \dots, z_n$) shows that the coefficient matrix M is non-singular, so that the above system in $x_1, x_2, \dots, x_N$ has a unique solution. As taking conjugate of every equation in the system produces the same system of equations in the variables $\overline{x_1}, \overline{x_2}, \dots, \overline{x_N}$, we conclude that all x_j are real. Therefore, we can take $c_j = 1$ and $d_j = x_j$, $j = 1, \dots, N$ in (5.1); the results of [16] now imply that the points z_k and $\overline{z_k}$ are eigenvalues of the operator H of multiplicity m_k, while Λ_0 is the common part of the spectra of the Hamiltonians H_0 and H. The proof is complete. □

Remark 5.2. As is clear from the proof of the main results, there are infinitely many $\mathcal{PT}$-symmetric rank-one perturbations of H_0 producing the desired spectral effect; e.g., in the above proof, the Fourier coefficients a_k and b_k of φ and ψ in (2.3) are determined only up to fixing their product $a_k b_k$.

Example 5.3. *Take H_0 to be the quantum harmonic oscillator (in dimensionless coordinates)*

$$H_0 = -\frac{d^2}{dx^2} + x^2$$

in the Hilbert space $\mathcal{H} = L_2(\mathbb{R})$. As is well known [37, Ch.8.3], the bound states of H_0 are $\lambda_n = 2n + 1$, $n \geq 0$, and the corresponding normalized eigenfunctions are

$$v_n(x) = \frac{\pi^{-1/4}}{\sqrt{2^n n!}} H_n(x) e^{-x^2/2},$$

with H_n being the n^{th} Hermite polynomial. Let also $\mathcal{P}$ and $\mathcal{T}$ be the standard space parity and time reversal operators in $\mathcal{H}$.

With the notations fixed at the beginning of this section, we set $\mu_j = 2j - 1$ and $w_j = v_{j-1}$, $j = 1, \ldots, N$. Solving the system of N linear equations generated by the equalities (5.2)*, we get real values for the variables $x_1, x_2, \ldots, x_N$, then choose real c_j and d_j satisfying $c_j d_j = x_j$, and, finally, construct the functions φ and ψ via* (5.1)*.*

The corresponding rank-one perturbation

$$H = -\frac{d^2}{dx^2} + x^2 + \langle \cdot, \varphi \rangle \psi$$

of H_0 is $\mathcal{PT}$-symmetric, has non-real eigenvalues at the points z_k and $\overline{z}_k$ of multiplicity m_k, $k = 1, 2, \ldots, n$, and the remaining eigenvalues and eigenfunctions are $\mu_j := 2j+1$ and v_j, $j \geq N$, as in the initial H_0.

6. Discussion and conclusion

The main results of the paper show that, given an arbitrary self-adjoint $\mathcal{PT}$-symmetric Hamiltonian H_0 with discrete spectrum, any finite subset of its eigenvalues can be moved by a $\mathcal{PT}$-symmetric rank-one perturbation into any desired collection of complex conjugate pairs, each with any desired degeneracy. It should be noted that, in fact, H_0 need not have purely discrete spectrum and that a continuous spectrum component may co-exist with bound states. The explicit constructions suggested in Theorem 5.1 can be accommodated to the spectral subspace corresponding to the discrete spectrum.

In this paper, we have not discussed what changes a $\mathcal{PT}$-symmetric rank-one perturbation may have on the spectrum of H_0 globally, for instance, what are possible asymptotics of the bound state distribution. This question requires different analytic tools and will be addressed in a separate research.

Finally, an interesting observation is that for every $\mathcal{PT}$-symmetric Hamiltonian H_1 with finite non-real spectrum there is a Hermitian $\mathcal{PT}$-symmetric Hamiltonian H_0 and its rank-one $\mathcal{PT}$-symmetric perturbation H such that H and H_1 possess the same spectra counting with multiplicities. To construct H_0 explicitly, we denote by N the total multiplicity of the non-real spectrum of H_1 and by $\{\lambda_k\}$ its real bound states. We then augment $\{\lambda_k\}$ with arbitrary N real values λ'_j, $j = 1, 2, \ldots, N$, denote the union by $\{\mu_n\}$, take an orthonormal basis of $\mathcal{H}$ consisting of $\mathcal{PT}$-symmetric functions v_n, and construct H_0 through the spectral theorem with bound states μ_n and eigenfunctions v_n,

$$H_0 := \sum \mu_n \langle \, \cdot \, , v_n \rangle v_n.$$

Then we apply Theorem 5.1 to move the bound states λ'_j to non-real spectrum of H_1 by a suitably chosen rank-one $\mathcal{PT}$-symmetric perturbation resulting in a $\mathcal{PT}$-symmetric Hamiltonian H. It is an interesting open question, if H_0 can be chosen so that H coincides with H_1.

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