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Symmetries of ($N \times N$) non-Hermitian Hamiltonian matrices

A Alaña, S Martínez-Garaot, M A Simón and J G Muga

Department of Physical Chemistry, UPV/EHU, Bilbao 48080, Spain

E-mail: jg.muga@ehu.es

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Abstract

A non-Abelian group of 16 symmetry operations on (generally) non-Hermitian discrete Hamiltonians represented by $N \times N$ matrices is studied. The symmetry operations are described by unitary/antiunitary superoperators that arise when combining three basic generating operations with simple 'geometric' interpretations. The corresponding Hamiltonian symmetries occur when the Hamiltonian remains invariant under the superoperator action. These symmetries include PT-symmetry and Hermiticity as particular cases. The interplay between the group of symmetry operations and Hamiltonian symmetries is analyzed systematically by introducing the concepts of equivalent operations and associated symmetries. Spectral properties implied by some of the symmetries are described.

Keywords: non Hermitian physics, PT—symmetry, group theory

(Some figures may appear in colour only in the online journal)

1. Introduction

Non-Hermitian Hamiltonians have been used for a long time in nuclear, atomic, and molecular physics as effective interactions, and have become common in optics, a field in which the wave equations in waveguides mimic quantum Schrödinger equations [1–3]. Non-Hermitian effective Hamiltonians may be constructed phenomenologically, in particular to describe gain and loss, see e.g. [1], or be derived from a more fundamental Hermitian Hamiltonian by projecting on a subspace [4–6].

In recent times PT-symmetric Hamiltonians [7] have attracted much attention because of interesting and useful spectral or scattering properties and many applications [2, 3], but recent work points at alternative symmetries [8–13] and even to a natural systematization of symmetry operations with a group structure [11]. In [13] an Abelian E8 group was described for symmetry operations on 'scattering Hamiltonians' that drive a particle state scattered off a potential center in one dimension (1D). It was shown there that devices for asymmetric response forbidden by PT-symmetry, such as a Maxwell demon, are compatible with some alternative symmetries. The present paper aims at extending the systematization of symmetry operations to discrete and finite Hamiltonian matrices, for which a larger non-Abelian group of 16 symmetry operations emerges naturally.

After reviewing briefly the results for scattering systems and pointing out the differences with discrete finite matrices in the remaining part of the Introduction, we shall describe the symmetry operations by means of superoperators in section 2; study the group of symmetry operations in section 3; its relation to actual Hamiltonian symmetries in section 4; and spectral properties in section 5. The paper ends with the conclusions and a discussion on open questions.

1.1. Scattering Hamiltonians (review)

A strong motivation to study non-Hermitian, one-dimensional (1D) scattering Hamiltonians $H = H_0 + V$[1], is the need to design devices with asymmetrical response, 'asymmetrical devices' for short [11], for particles or waves incident from both sides, such as diodes, valves, or rectifiers. We may expect many applications of asymmetrical devices in optics or the microscopic world, in quantum information processing and other quantum technologies.

Ruschhaupt *et al* [11] describe six types of asymmetrical devices according to their transmission and reflection coefficients, and their relation, in the form of selection rules, to eight different symmetries that H could fulfill with the forms

$$AH = HA, \tag{1}$$

$$AH = H^\dagger A, \tag{2}$$

where A is a unitary or antiunitary operator in the Klein four-group $K_4 = \{1, \Pi, \theta, \Pi\theta\}$ [11]. If (2) is fulfilled we say that H is A-pseudo-Hermitian [11, 14]. The operators Π, θ and $\Pi\theta$ of the K_4 group are parity, time reversal (for a spinless particle) and the consecutive (commuting) application of both. Their properties are well known but we review them quickly for comparison with later, different usage of the symbols:

- Π: in the continuous space the parity operator is a linear, unitary operator that inverts the position vector across the origin, so that $\Pi c|x\rangle = c|-x\rangle$ for a complex number c. Also, $\Pi^2 = 1$.
- θ: in the continuous space it is the 'temporal inversion', an antilinear, antiunitary operator that on a spinless-particle state acts in coordinate and momentum representations as follows,

$$\theta \int \mathrm{d}x|x\rangle\langle x|\psi\rangle = \int \mathrm{d}x|x\rangle\langle\psi|x\rangle, \tag{3}$$

$$\theta \int \mathrm{d}p|p\rangle\langle p|\psi\rangle = \int \mathrm{d}p|-p\rangle\langle\psi|p\rangle, \tag{4}$$

so that $\theta\theta = 1$.

[1] $H_0 = p^2/(2m)$ is the kinetic energy for a non relativistic particle of mass m, p being the momentum, and V is the potential, which is assumed to decay fast enough on both sides to have a continuous spectrum and scattering eigenfunctions.

Table 1. (i) Roman number code that may represent the operation or the symmetry. (ii)Result of performing eight symmetry operations on H. (iii) Corresponding symmetries of the types (1) or (2). When H is invariant under the operation, the matrix elements of H obey these relations, and viceversa.

i	ii	iii
I	H	$\langle x\|H\|y\rangle = \langle x\|H\|y\rangle$
II	$H^\dagger$	$\langle x\|H\|y\rangle = \langle y\|H\|x\rangle^*$
III	$\Pi H\Pi$	$\langle x\|H\|y\rangle = \langle -x\|H\| - y\rangle$
IV	$\Pi H^\dagger\Pi$	$\langle x\|H\|y\rangle = \langle -y\|H\| - x\rangle^*$
V	$\theta H\theta$	$\langle x\|H\|y\rangle = \langle x\|H\|y\rangle^*$
VI	$\theta H^\dagger\theta$	$\langle x\|H\|y\rangle = \langle y\|H\|x\rangle$
VII	$\Pi\theta H\Pi\theta$	$\langle x\|H\|y\rangle = \langle -x\|H\| - y\rangle^*$
VIII	$\Pi\theta H^\dagger\Pi\theta$	$\langle x\|H\|y\rangle = \langle -y\|H\| - x\rangle$.

– $\Pi\theta$: it is also antilinear and antiunitary since the product of a linear operator and an antilinear operator is antilinear. Π and θ commute. It is also often called '*PT*'.

Combining the two possible relations (1) and (2), and the four A in Klein's group, we get the eight symmetries in [11] made explicit in table 1, column iii. They may be regarded as the invariance of the Hamiltonian with respect to corresponding eight symmetry operations that form the Abelian group E8 [13], see column ii.

As pointed out first for Hamiltonians with discrete spectrum by Mostafazadeh [15–17] and later extended to scattering Hamiltonians in [13], A-pseudo-Hermiticity with A linear, or the commutation of A and H for A antilinear imply that the eigenvalues of H come in conjugate pairs necessarily, in particular they may be real. These conditions occur for symmetries II, IV, V, and VII. No other symmetry in this set of eight or in the extension to 16 symmetries considered below satisfies them.

Let us emphasize and insist on the important distinction between *symmetry operations* on and *symmetries* of an operator or of the corresponding matrix. Symmetry operations are changes imposed to an operator or matrix, e.g. transformations such as taking the complex conjugate, or performing the transpose. An operator or matrix possesses a particular symmetry if the corresponding symmetry operation keeps the operator or matrix *invariant*. The roman number code in column i of table 1 will refer indistinctly to an operation or to a symmetry, the context should clarify the possible ambiguity.

1.2. $N \times N$ Hamiltonian matrices

The above analysis has to be extended when dealing with discrete Hamiltonians represented by $N \times N$ finite matrices in some orthonormal basis, such as the ones used to describe two-level, three-level, or N-level systems in simplified models of atomic structure or of artificial atoms in solid state physics or in optics. In this work it is assumed that the discrete Hamiltonians[2] are diagonalizable,

$$H = \sum_i |\phi_i\rangle E_i \langle\widehat{\phi_i}|, \tag{5}$$

[2] By default a 'discrete' basis or matrix is always finite here.

where the right, $|\phi_i\rangle$, and left eigenvectors, $\langle\widehat{\phi_i}|$, are biorthogonal partners, and E_i may be a complex number. These vectors form a biorthogonal basis such that $1 = \sum_i |\phi_i\rangle\langle\widehat{\phi_i}|$ and $\langle\widehat{\phi_i}|\phi_j\rangle = \delta_{ij}$.

To study the possible symmetries and symmetry operations for discrete Hamiltonians we shall first reset the meaning of the operators Π, θ, and $\Pi\theta$ to adapt them to a discrete orthonormal basis. They will stand now as 'geometrical' operators in a given basis as follows (more on this geometrical aspect in section 3.2 below):

– Π: for a finite orthonormal basis with basis states $|1\rangle, |2\rangle, ..., |N\rangle$, labeled by natural numbers, it transforms (linearly) the ith member of the basis to $-i$, $\Pi c|i\rangle = c|-i\rangle$, where $-i$ implies the 'opposite' of i with respect to the middle value of the basis index, i.e.

$$|-i\rangle \equiv |N+1-i\rangle. \tag{6}$$

Example: for a basis $\{|1\rangle, |2\rangle, |3\rangle\}$, $N = 3$ so $|-1\rangle = |3\rangle, |-3\rangle = |1\rangle$, and $|-2\rangle = |2\rangle$. (A basis could also have an even number of states and a half-integer middle value.) Π is a unitary operator. We may also regard it as a 'reflection' operator.

– θ: in the discrete basis, it will be an antilinear, antiunitary operator defined by $\theta c|j\rangle = c^*\theta|j\rangle = c^*|j\rangle$, where c is any complex constant.

– $\Pi\theta = \theta\Pi$: it is antilinear and antiunitary.

Note that in both discrete and continuous models, the operators Π, θ, and $\Pi\theta$ are their own inverses, and also Hermitian operators.

Since the structure of a discrete Hamiltonian does not have the limitations imposed by the properties of the kinetic energy Hamiltonian H_0 in the scattering form $H = H_0 + V$, a larger group of 16 symmetry operations that could leave the Hamiltonian invariant is found compared to the symmetry operations on scattering Hamiltonians, see table 2. The new operations with respect to those in table 2, from *IX* to *XVI*, imply to invert one of the kets but not the other one, applying parity only on one side. The corresponding symmetries do not have the forms (1) or (2).

This work is devoted to study the group of 16 symmetry operations and their relations with actual Hamiltonian symmetries. Before discussing properties of the abstract group we shall introduce its realization based on superoperators and their geometrical interpretation.

2. Superoperators

Different superoperator types are used in the group of 16 in table 2.

Let us define first superoperators $\mathcal{L}_{A,B}$ by left multiplying by A and right multiplying by B,

$$\mathcal{L}_{A,B}H = AHB. \tag{7}$$

Note that $\mathcal{L}_{A,B}H = H \iff A^{-1}H = HB$. We consider only $\mathcal{L}_{A,B}$ where both A and B are linear or both are antilinear, so as to preserve the linearity of a Hamiltonian. Otherwise $\mathcal{L}_{A,B}$ could not represent a symmetry. For example, the superoperator $\mathcal{L}_{1,\theta}$ creates an antilinear operator $\mathcal{L}_{1,\theta}H = H\theta$, so it is not in the group of 16 transformations. The operators A, B to construct the superoperator group will be chosen among Klein's group operators 1, Π, θ, and $\theta\Pi$, defined for a finite basis.

A shorthand notation $\mathcal{L}_A$ is used for $\mathcal{L}_{A^{-1},A}$,

$$\mathcal{L}_A H = A^{-1}HA, \tag{8}$$

Table 2. Group elements (transformations) in different notations. 1: roman number code; 2: group theory notation of group elements in terms of generators x, y, a, see (18) and (19); 3: superoperators $\mathcal{S}$; 4: explicit action of the superoperators on H; 5: geometrical interpretation of the symmetry operations, where—is the horizontal axis, | the vertical axis, \ is the main diagonal, / is the secondary diagonal, and cc is complex conjugation; 6: matrix element $\langle i|(\mathcal{S}H)|j\rangle$. A Hamiltonian symmetry occurs if $\langle i|(\mathcal{S}H)|j\rangle = \langle i|H|j\rangle$ for all i, j.

1	2	3	4	5	6
I	e	$\mathcal{L}_1$	H	Do nothing	$\langle i\|H\|j\rangle$
II	x	$\mathcal{D}$	$H^\dagger$	Flip along \ and cc	$\langle j\|H\|i\rangle^*$
III	a^2	$\mathcal{L}_\Pi$	$\Pi H\Pi$	Rotate by π	$\langle -i\|H\|-j\rangle$
IV	xa^2	$\mathcal{L}_\Pi\mathcal{D}$	$\Pi H^\dagger\Pi$	Flip along / and cc	$\langle -j\|H\|-i\rangle^*$
V	y	$\mathcal{L}_\theta$	$\theta H\theta$	cc	$\langle i\|H\|j\rangle^*$
VI	xy	$\mathcal{L}_\theta\mathcal{D}$	$\theta H^\dagger\theta$	Flip along \	$\langle j\|H\|i\rangle$
VII	a^2y	$\mathcal{L}_{\Pi\theta}$	$\Pi\theta H\Pi\theta$	Rotate by π and cc	$\langle -i\|H\|-j\rangle^*$
VIII	a^2xy	$\mathcal{L}_{\Pi\theta}\mathcal{D}$	$\Pi\theta H^\dagger\Pi\theta$	Flip along /	$\langle -j\|H\|-i\rangle$
IX	$ax = xa^3$	$\mathcal{L}_{1,\Pi}$	$H\Pi$	Flip along |	$\langle i\|H\|-j\rangle$
X	$xa = a^3x$	$\mathcal{L}_{\Pi,1}$	ΠH	Flip along—	$\langle -i\|H\|j\rangle$
XI	axy	$\mathcal{L}_\theta\mathcal{L}_{1,\Pi}$	$\theta H\theta\Pi$	Flip along | and cc	$\langle i\|H\|-j\rangle^*$
XII	a^3xy	$\mathcal{L}_\theta\mathcal{L}_{\Pi,1}$	$\Pi\theta H\theta$	Flip along—and cc	$\langle -i\|H\|j\rangle^*$
XIII	a	$\mathcal{L}_{1,\Pi}\mathcal{D}$	$H^\dagger\Pi$	Rotate by $\pi/2$ and cc	$\langle -j\|H\|i\rangle^*$
XIV	a^3	$\mathcal{L}_{\Pi,1}\mathcal{D}$	$\Pi H^\dagger$	Rotate by $3\pi/2$ and cc	$\langle j\|H\|-i\rangle^*$
XV	$ay = ya$	$\mathcal{L}_\theta\mathcal{L}_{1,\Pi}\mathcal{D}$	$\theta H^\dagger\Pi\theta$	Rotate by $\pi/2$	$\langle -j\|H\|i\rangle$
XVI	a^3y	$\mathcal{L}_\theta\mathcal{L}_{\Pi,1}\mathcal{D}$	$\theta\Pi H^\dagger\theta$	Rotate by $3\pi/2$	$\langle j\|H\|-i\rangle$

where A^{-1} is the inverse of A. It is easily seen that $\mathcal{L}_A H = H \iff [H, A] = 0$.

To complete the 16 operations we also define a 'dagger' superoperator $\mathcal{D}$ that transforms an operator into its adjoint [12],

$$\mathcal{D}H = H^\dagger. \tag{9}$$

Hermiticity is the symmetry that corresponds to invariance upon this superoperator.

It is possible to combine the former superoperators applying them sequentially to find new ones [12], for example,

$$\mathcal{L}_A\mathcal{D}H = A^{-1}H^\dagger A, \tag{10}$$

$$\mathcal{D}\mathcal{L}_A H = (A^{-1}HA)^\dagger. \tag{11}$$

$\mathcal{L}_A\mathcal{D}H = H \iff AH = H^\dagger A$. In general $\mathcal{L}_A\mathcal{D}H \neq \mathcal{D}\mathcal{L}_A H$, but $\mathcal{L}_A$ and $\mathcal{D}$ commute when $A^{-1} = A^\dagger$, as it happens for our basic operators 1, Π, θ and $\theta\Pi$ in Klein's group.

The group of superoperators that preserve linearity are given in columns 3 and 4 of table 2. A sense of 'completeness' of the 16 operations is discussed below in section 3.2 from a geometrical perspective. As before the roman numbers in column 1 are conventional indices for operations and/or symmetries, and when the matrix element in the rightmost column 6 equals $\langle i|H|j\rangle$, H is invariant under the transformation and posseses a symmetry. It proves convenient to denote an arbitrary superoperator in this group by a generic notation $\mathcal{S}$. In formal manipulations we shall later on use distinguishing subscripts, e.g. $\mathcal{S}_j$, where $j = 1, 2, ..., 16$ mapping $I \to 1$, $II \to 2$, etc...

Superoperators, just like ordinary operators, are linear if they leave complex constants invariant and antilinear if they transform them to their complex conjugates. In particular [12],

$$
\begin{aligned}
\mathcal{L}_A(cH) &= cA^\dagger HA, \quad A \text{ unitary}, \\
\mathcal{L}_A(cH) &= c^* A^\dagger HA, \ A \text{ antiunitary}, \\
\mathcal{L}_{A,B}(cH) &= cAHB, \quad A \text{ and } B \text{ unitary}, \\
\mathcal{L}_{A,B}(cH) &= c^* AHB, \quad A \text{ and } B \text{ antiunitary}, \\
\mathcal{D}(cH) \quad &= c^* H^\dagger, \\
\mathcal{L}_A\mathcal{D}(cH) &= \mathcal{D}\mathcal{L}_A(cH) = c^* A^\dagger H^\dagger A, \ A \text{ unitary}, \\
\mathcal{L}_A\mathcal{D}(cH) &= \mathcal{D}\mathcal{L}_A(cH) = cA^\dagger H^\dagger A, A \text{ antiunitary}.
\end{aligned}
\tag{12}
$$

2.1. Valid symmetry operations

The transformations considered in quantum physics as possible symmetries, i.e. symmetry transformations (operations), are not really arbitrary. Wigner set the rule that they should leave the modulus of the scalar product of two states, equivalently their ‘transition probability’, invariant, and this restricts the corresponding operators to be unitary or antiunitary [18]. As seen below in detail, our superoperators imply a mild generalization of Wigner’s definition, as they leave the scalar product of two density operators, which constitute the most general way of expressing a state, invariant.

We will denote a scalar product of two given (linear) operators F and G as $\langle\langle F, G\rangle\rangle$. The general expression of the scalar product of two linear operators is $\langle\langle F, G\rangle\rangle = \mathrm{Tr}(F^\dagger G)$ [12]. Expectation values for an observable F and a density operator ρ, both Hermitian, take the form $\langle F\rangle = \mathrm{Tr}[F\rho] = \mathrm{Tr}[F^\dagger\rho] = \langle\langle F, \rho\rangle\rangle$.

Now, we can define the adjoint of a given superoperator $\mathcal{S}$ as the superoperator $\mathcal{S}^\dagger$ which fulfills [12]

$$
\langle\langle G, \mathcal{S}F\rangle\rangle = \langle\langle F, \mathcal{S}^\dagger G\rangle\rangle^* \ \text{ for } \mathcal{S} \text{ linear}, \tag{13}
$$

$$
\langle\langle G, \mathcal{S}F\rangle\rangle = \langle\langle F, \mathcal{S}^\dagger G\rangle\rangle \ \text{ for } \mathcal{S} \text{ antilinear}. \tag{14}
$$

For unitary or antiunitary operators A, so $A^{-1} = A^\dagger$, we find [12]

$$
\begin{aligned}
\mathcal{L}_A^\dagger(\cdot) &= \mathcal{L}_{A^\dagger}(\cdot) \equiv A(\cdot)A^\dagger, \\
\mathcal{D}^\dagger(\cdot) &= \mathcal{D}(\cdot), \\
(\mathcal{L}_A\mathcal{D})^\dagger(\cdot) &= \mathcal{L}_{A^\dagger}\mathcal{D}(\cdot).
\end{aligned}
\tag{15}
$$

For a more general $\mathcal{L}_{A,B}$, with A and B both unitary or aniunitary, $\mathcal{L}_{A,B}^\dagger = \mathcal{L}_{A^\dagger B^\dagger}$. This is easy to check when A and B are both unitary,

$$
\begin{aligned}
&\langle\langle F, \mathcal{L}_{A,B}^\dagger G\rangle\rangle = \langle\langle G, \mathcal{L}_{A,B}F\rangle\rangle^* \\
&= \mathrm{Tr}[(G^\dagger AFB)^\dagger] = \mathrm{Tr}[B^\dagger F^\dagger A^\dagger G] \\
&= \mathrm{Tr}[F^\dagger A^\dagger GB^\dagger], \text{ using cyclic permutation}.
\end{aligned}
\tag{16}
$$

For antiunitary A and B, $\mathcal{L}_{A,B}$ is antiunitary and the calculation is more elaborate but the result is the same.

For all 16 superoperators an explicit calculation gives $\mathcal{S}^{\dagger} = \mathcal{S}^{-1}$, so these superoperators are unitary or antiunitary. This is clear in the set (15) and for $\mathcal{L}_{A,B}$ it is also true because we only consider A and B to be simultaneously unitary or antiunitary. Thus $\mathcal{L}_{A,B}\mathcal{L}_{A^{\dagger}B^{\dagger}}F = AA^{\dagger}FB^{\dagger}B = F$, and similarly $\mathcal{L}_{A^{\dagger}B^{\dagger}}\mathcal{L}_{A,B}F = F$.

Parallel to the fact that a unitary or antiunitary operator A keeps the scalar product of two states represented by kets invariant ($|\psi_1\rangle, |\psi_2\rangle \Rightarrow \langle\psi_1|\psi_2\rangle; A|\psi_1\rangle, A|\psi_2\rangle \Rightarrow \langle\psi_1|A^{\dagger}A|\psi_2\rangle = \langle\psi_1|\psi_2\rangle$), unitary and antiunitary superoperators keep invariant the scalar product of two density operators,

$$\langle\langle\rho_1, \rho_2\rangle\rangle = \langle\langle\mathcal{S}\rho_1, \mathcal{S}\rho_2\rangle\rangle. \tag{17}$$

This property defines, extending Wigner's approach to symmetry [19], a symmetry transformation.

3. Study of the group

The set of 16 superoperators (symmetry operations) has a group structure, it may be considered as the direct product of the dihedral group D8 and the cyclic group Z2 and has many subgroups that we shall briefly discuss. To the best of our knowledge the group is not known by any particular name, so we shall call it G_{16} for short. The abstract group in our case is realized by all transformations that can be performed on a discrete Hamiltonian matrix making use of complex conjugation, transposition, and inversion of one or two states in the matrix element. This is a group of *symmetry operations* on the Hamiltonian matrices, not necessarily the group of symmetries of a given Hamiltonian.

3.1. Structure of the group

3.1.1. Group of 16 transformations. G_{16} is not Abelian. Not all the elements of the group commute with each other, even thought some of them do. We also notice that most of the elements are their own inverses, except XIII, XIV, XV, and XVI. Their inverse is the application of themselves three times, $(\mathcal{L}_{1,\Pi}\mathcal{D})^{-1} = (\mathcal{L}_{1,\Pi}\mathcal{D})^3$, and $(\mathcal{L}_{\Pi,1}\mathcal{D})^{-1} = (\mathcal{L}_{\Pi,1}\mathcal{D})^3$. We have thus operations of order 2 or 4 in the group, the order here being the minimal number of times needed to get the identity by successive application of the same superoperator.

The 'presentation' of the abstract group G_{16}, which summarizes its properties and relations among elements is given, in group theory notation (not to be confused with a quantum scalar product) by

$$\langle a, y, x \mid a^4 = x^2 = y^2 = e, xax = a^{-1}, ya = ay, xy = yx\rangle. \tag{18}$$

This means that the group can be created by combining three generators, that we call x, y and a. e is the identity. In other words, every element of the group can be expressed as the combination under the group operation, which in our realization is implemented by applying the transformations successively, of finitely many elements of the subset $\{x, y, a\}$. The shorthand notation $\langle a, y, x\rangle$ represents the group G_{16}, and similarly different subgroups are represented in this way by specifying only the generators in $\langle ...\rangle$. The generators obey the relations on the right hand side of the presentation $\langle a, y, x| ....\rangle$. These relations combined produce many others such as $ax = xa^3$, $xa = a^3x$, $ax^2 = x^2a$, and suffice to construct the multiplication table of the group, see table 3. When e appears in the diagonal the corresponding superoperators are the inverse of each other. The ordering of operations to construct the matrix of the table is conventionally that the element in the ith row and jth column is given by $\mathcal{S}_{(i,j)} = \mathcal{S}_i\mathcal{S}_j$.

Different superoperators may play the role of generators, in particular we choose

$$\begin{aligned} &x \rightarrow \mathcal{D}, \\ &y \rightarrow \mathcal{L}_\theta, \\ &a \rightarrow \mathcal{L}_{1,\Pi}\mathcal{D}. \end{aligned} \tag{19}$$

The relation between the different notations used so far are given in table 2.

Remark on notation: the roman-number code has played a role to relate the present results to previous work in [11–13] and it makes clear that the eight symmetry operations discussed there may be generalized into a larger set of 16 transformations for finite matrices. However, a group-theory type of code (column 2 in table 2) is almost as compact but it carries considerably more information, so it is our notation of choice from now on.

3.1.2. Subgroups. According to Lagrange's theorem[3], the number of the elements in the subgroups are 1 (the identity), 2 (formed by the identity and members that are their own inverses), 4, and 8 [19]. There are no other possibilities.

A physically relevant subgroup is composed by the first eight superoperators, $\{e, x, a^2, a^2x, y, xy, a^2y, a^2xy\}$, this is the E8 group mentioned before [13]. A compact notation for this subgroup is $\langle x, y, a^2\rangle$, i.e. it is generated by x, y, and a^2. By contrast, G_{16} is $\langle a, y, x\rangle$. G_{16} can be generated by other combinations as well, for example $\langle a^3, y, x\rangle$, $\langle ya, x, y\rangle$, $\langle ya, y, xy\rangle$, etc...

This is the list of subgroups of order 8[4]:

- E8, $\langle x, y, a^2 \mid x^2 = y^2 = (a^2)^2 = e, xy = yx, a^2x = xa^2, a^2y = ya^2\rangle$.
- E8, $\langle ax, y, a^2 \mid (ax)^2 = y^2 = (a^2)^2 = e, xy = yx, a^2(ax) = (ax)a^2, a^2y = ya^2\rangle$
- Direct product of Z4 and Z2, $\langle a, y \mid a^4 = y^2 = e, ay = ya\rangle$.
- D8, $\langle a, x \mid a^4 = x^2 = e, xax^{-1} = a^{-1}\rangle$.
- D8, $\langle a, xy \mid a^4 = (xy)^2 = e, (xy)a(xy)^{-1} = a^{-1}\rangle$.
- D8, $\langle ay, x \mid (ay)^4 = x^2 = e, x(ay)x^{-1} = (ay)^{-1}\rangle$.
- D8, $\langle ay, ax \mid (ay)^4 = (ax)^2 = e, (ax)(ay)(ax)^{-1} = (ay)^{-1}\rangle$. This subgroup contains the unitary transformations.

Among the subgroups of order 4, we highlight two cyclic groups Z4. One is formed by $\{a, a^2, a^3, 1\}$, i.e. $\langle a\rangle$ (or $\langle a^3\rangle$ since repeated action of a^3 generates the same group), and the other one by $\{ya, a^2, ya^3, 1\}$, i.e. $\langle ya\rangle$ or $\langle ya^3\rangle$:

- Z4, $\langle a \mid a^4 = e, a^{-1} = a^3\rangle$.
- Z4, $\langle ay \mid (ay)^4 = e, (ay)^{-1} = (ay)^3\rangle$.

There are 13 other subgroups with four elements: $\langle a^2, x\rangle$, $\langle a^2, ax\rangle$, $\langle a^2, xy\rangle$, $\langle a^2, axy\rangle$, $\langle x, y\rangle$, $\langle y, ax\rangle$, $\langle y, a^2x\rangle$, $\langle y, a^3x\rangle$, $\langle a^2y, x\rangle$, $\langle a^2y, ax\rangle$, $\langle a^2y, a^2x\rangle$, $\langle a^2y, a^3x\rangle$, and $\langle a^2, y\rangle$, which is the 'center' (its elements commute with all elements). The full group of 16 may be constructed by direct product of different subgroups, for example we shall use later the product of $\langle x, y\rangle$ with any of the cyclic groups Z4, $\langle a\rangle$ or $\langle ay\rangle$.

[3] For any finite group G, the 'order' (now number of elements) of every subgroup of G divides the order of G.

[4] For other properties of the abstract group G_{16} see https://groupprops.subwiki.org/wiki/Direct_product_of_D8_and_Z2

Table 3. Multiplication table of G_{16}. The element of the column is applied first, then the one in the row, $\mathcal{S}_{\text{row}}\mathcal{S}_{\text{column}} = \mathcal{S}_{\text{table}}$. The bold area represents the table of the E8 group in [12].

	e	x	a^2	a^2x	y	xy	a^2y	a^2xy	ax	xa	axy	a^3xy	a	a^3	ya	a^3y
e	$\mathbf{e}$	$\mathbf{x}$	$\mathbf{a^2}$	$\mathbf{a^2x}$	$\mathbf{y}$	$\mathbf{xy}$	$\mathbf{a^2y}$	$\mathbf{a^2xy}$	ax	xa	axy	a^3xy	a	a^3	ya	a^3y
x	$\mathbf{x}$	$\mathbf{e}$	$\mathbf{a^2x}$	$\mathbf{a^2}$	$\mathbf{xy}$	$\mathbf{y}$	$\mathbf{a^2xy}$	$\mathbf{a^{2y}}$	a^3	a	a^3y	ya	xa	ax	a^3xy	axy
a^2	$\mathbf{a^2}$	$\mathbf{a^2x}$	$\mathbf{e}$	$\mathbf{x}$	$\mathbf{a^2y}$	$\mathbf{a^2xy}$	$\mathbf{y}$	$\mathbf{xy}$	xa	ax	a^3xy	axy	a^3	a	a^3y	ya
a^2x	$\mathbf{a^2x}$	$\mathbf{a^2}$	$\mathbf{x}$	$\mathbf{e}$	$\mathbf{a^2xy}$	$\mathbf{a^2y}$	$\mathbf{xy}$	$\mathbf{y}$	a	a^3	ya	a^3y	ax	xa	axy	a^3xy
y	$\mathbf{y}$	$\mathbf{xy}$	$\mathbf{a^2y}$	$\mathbf{a^2xy}$	$\mathbf{e}$	$\mathbf{x}$	$\mathbf{a^2}$	$\mathbf{a^2x}$	axy	a^3xy	ax	xa	ya	a^3y	a	a^3
xy	$\mathbf{xy}$	$\mathbf{y}$	$\mathbf{a^2xy}$	$\mathbf{a^2y}$	$\mathbf{x}$	$\mathbf{e}$	$\mathbf{a^2x}$	$\mathbf{a^2}$	a^3y	ya	a^3	a	a^3xy	axy	xa	ax
a^2y	$\mathbf{a^2y}$	$\mathbf{a^2xy}$	$\mathbf{y}$	$\mathbf{xy}$	$\mathbf{a^2}$	$\mathbf{a^2x}$	$\mathbf{e}$	$\mathbf{x}$	a^3xy	axy	xa	ax	a^3y	ya	a^3	a
a^2xy	$\mathbf{a^2xy}$	$\mathbf{a^{2y}}$	$\mathbf{xy}$	$\mathbf{y}$	$\mathbf{a^2x}$	$\mathbf{a^2}$	$\mathbf{x}$	$\mathbf{e}$	ya	a^3y	a	a^3	axy	a^3xy	ax	xa
ax	ax	a	xa	a^3	axy	ya	a^3xy	a^3y	e	a^2	y	a^2y	x	a^2x	xy	a^2xy
xa	xa	a^3	ax	a	a^3xy	a^3y	axy	ya	a^2	e	a^2y	y	a^2x	x	a^2xy	xy
axy	axy	ya	a^3xy	a^3y	ax	a	xa	a^3	y	a^2y	e	a^2	xy	a^2xy	x	a^2x
a^3xy	a^3xy	a^3y	axy	ya	xa	a^3	ax	a	a^2y	y	a^2	e	a^2xy	xy	a^2x	x
a	a	ax	a^3	xa	ya	axy	a^3y	a^3xy	a^2x	x	a^2xy	xy	a^2	e	a^2y	y
a^3	a^3	xa	a	ax	a^3y	a^3xy	ya	axy	x	a^2x	xy	a^2xy	e	a^2	y	a^2y
ya	ya	axy	a^3y	a^3xy	a	ax	a^3	xa	a^2xy	xy	a^2x	x	a^2y	y	a^2	e
a^3y	a^3y	a^3xy	ya	axy	a^3	xa	a	ax	xy	a^2xy	x	a^2x	y	a^2y	e	a^2

How large is the group generated by one or two group elements? If we choose a single operation to create a group, other than the identity, the group will have four elements for operations that are not their own inverse (elements of order 4, namely a,a^3,ay, and a^3y). Otherwise, the group will have only two elements, the operation and the identity.

Two distinct elements can generate groups with two, four, or eight elements:

– Two elements if one of them is e and the other one is its own inverse.

If neither of them is the identity,

– Four elements if they commute, excluding the combination of a member of order 4 and a member not in the cycles Z4 (for example a and y generate a group of order 8).
– Eight elements for all other pairs, in particular the ones that do not commute, and the combinations of an element of order 4 and elements that do not belong to the cycles $Z4$.

3.2. Geometrical interpretation

All 16 operations on the matrix elements may be viewed as geometrical operations on the matrix elements, including complex conjugation. There are several generating operations we can choose, but a simple choice for visualization purposes is the following, see also figure 1:

(i) ya: rotate the matrix by $\pi/2$.
(ii) y: take the complex conjugate.
(iii) xy: invert (flip) the matrix with respect to the main diagonal.

They fulfill $\langle xy, y, ya\rangle = G_{16}$, which means that with these three operations combined we can find all operations, which include, in geometrical language, axial flips along perpendicular horizontal or vertical bisectors, and axial flips along the perpendicular diagonals, as well as rotations by $3\pi/2$, all of them with or without complex conjugation. The explicit geometrical interpretation of all symmetry operations is given in table 2, column 5.

Figure 1 shows the structure of 2×2 matrices that posses each of the 16 symmetries. Different symbols indicate different complex numbers. The same symbol without a point and with a point inside represent a complex number and its complex conjugate. Finally, filled symbols represent real numbers.

The reader may notice that the symmetries XIII and XIV are special in that they imply the same matrix structure, as it also happens to symmetries XV and XVI. Here the distinction between symmetry operation and symmetry is quite crucial: whereas the symmetry operations XIII and XIV (or XV and XVI) are distinct, the corresponding symmetries imply each other and hold under the same conditions for the matrix elements. This special relation is explained in detail in the following section.

4. Implications of one or more symmetries of the Hamiltonian

4.1. Equivalence of symmetry operations and associated symmetries

The ‘symmetries of H’ necessarily form a subgroup G_{SH} with group structure, as the consecutive application of two superoperators that leave H invariant will also leave H invariant. This section explores the interplay between G_{16} and G_{SH}, specifically the consequences of some existing symmetry. To that end we introduce two concepts: equivalent operations and associated symmetries.

We will say that, *conditioned to an existing symmetry or set of symmetries* $\{\mathcal{S}_iH = H, \mathcal{S}_jH = H, ...\}$, two symmetry operations represented by $\mathcal{S}_k$ and $\mathcal{S}_l$ are equivalent, $\mathcal{S}_k \sim \mathcal{S}_l$ (more explicitly, $\mathcal{S}_k \sim \mathcal{S}_l | \{\mathcal{S}_iH = H, \mathcal{S}_jH = H, ...\}$) if $\mathcal{S}_kH = \mathcal{S}_lH$.

$\mathcal{S}_k \sim \mathcal{S}_l$ is indeed an equivalence relation in mathematical sense since it is reflexive (a given superoperator is equivalent to itself); symmetric (if $\mathcal{S}_k \sim \mathcal{S}_l$, then $\mathcal{S}_l \sim \mathcal{S}_k$); and transitive (if $\mathcal{S}_k \sim \mathcal{S}_l$, and $\mathcal{S}_l \sim \mathcal{S}_m$, then $\mathcal{S}_k \sim \mathcal{S}_m$).

Equivalence relations provide partitions of the groups into equivalence classes. In the G_{16} group, each class is given by the superoperators that are equivalent to each other. One of these classes is the group G_{SH}: all symmetry operations that leave the Hamiltonian invariant are equivalent among themselves and to the identity $\mathcal{L}_I$.

Equivalent pairs are easily found using the multiplication table of the group. If $\mathcal{S}_iH = H$, then $\mathcal{S}_j = \mathcal{S}_k\mathcal{S}_i$ (read from the table) and $\mathcal{S}_k$ are equivalent.

An example of equivalence that may be familiar to some is that, conditioned on $xyH = H$ (which is satisfied in particular by all local potentials if we consider scattering Hamiltonians in coordinate representation; more generally this symmetry implies that the matrix is complex-symmetric or, equivalently, self-transpose), then $a^2yH = a^2xH$. In the alternative operator language this means that, conditioned on $\theta H^\dagger\theta = H$, we have that $\Pi\theta H\Pi\theta = \Pi H^\dagger\Pi$. In words, with the proper conditioning (θ-pseudo-Hermiticity, i.e. the symmetry of complex-symmetric matrices), the symmetry transformations related to PT-symmetry and to parity-pseudo-Hermiticity give the same result when acting on the Hamiltonian. If it happens that H is indeed PT-symmetrical (i.e. $\Pi\theta H\Pi\theta = H$), then it will also be parity-pseudo-Hermitian ($\Pi H^\dagger\Pi = H$) and viceversa [14, 20]. These symmetry pairs were explored systematically in [11] within the E8 group $\langle x, y, a^2\rangle$ studied there, conditioned on a given (primary) symmetry. The novelty in the present work is twofold: we extend the analysis to G_{16} and also define the equivalence relation more precisely, as a relation among symmetry operations acting on H: as here defined, the equivalent pair is not necessarily a pair of Hamiltonian symmetries, but a pair of operations that, when acting on H, give the same result.

Two symmetry operations represented by $\mathcal{S}_i$ and $\mathcal{S}_j$ are associated symmetry operations if $\mathcal{S}_i \in G_{SH} \iff \mathcal{S}_j \in G_{SH}$. In our group the two elements of order 4 in a given subgroup Z4 are associated symmetries: a and a^3 are associated, as well as ay and a^3y. The bidirectionality is important. For example $a \in G_{SH} \Rightarrow a^2 \in G_{SH}$ but the reverse does not hold, so a and a^2 are not associated symmetries. Two associated symmetries imply the same structure on the Hamiltonian, i.e. the relations that the matrix elements satisfy are equal in both cases, as illustrated in figure 1.

Association is a stronger relation than equivalence since it implies equivalence, but equivalence does not imply association.

4.1.1. Effects of one non-trivial symmetry of the Hamiltonian. For the following discussion some additional terminology is needed: a 'symmetry or order n' represents the invariance of the Hamiltonian with respect to a superoperator of order n (where n is the minimal power $n \geqslant 1$ of the superoperator that gives the identity).

Symmetry of order 2. Suppose that H is invariant under x, $xH = H$. Since $x^2 = e$, the group composed by x and e is in G_{SH} (It might even be the full G_{SH} if there are no other symmetries). Acting with y on x we have that

$$yxH = y(xH) = yH, \tag{20}$$

so $yx \sim y$ conditioned on $xH = H$. In fact there is nothing special about y here. We can premultiply x by the 16 members of the group, to get 16 superoperators $\mathcal{S}_jx = \mathcal{S}_k$. If the index

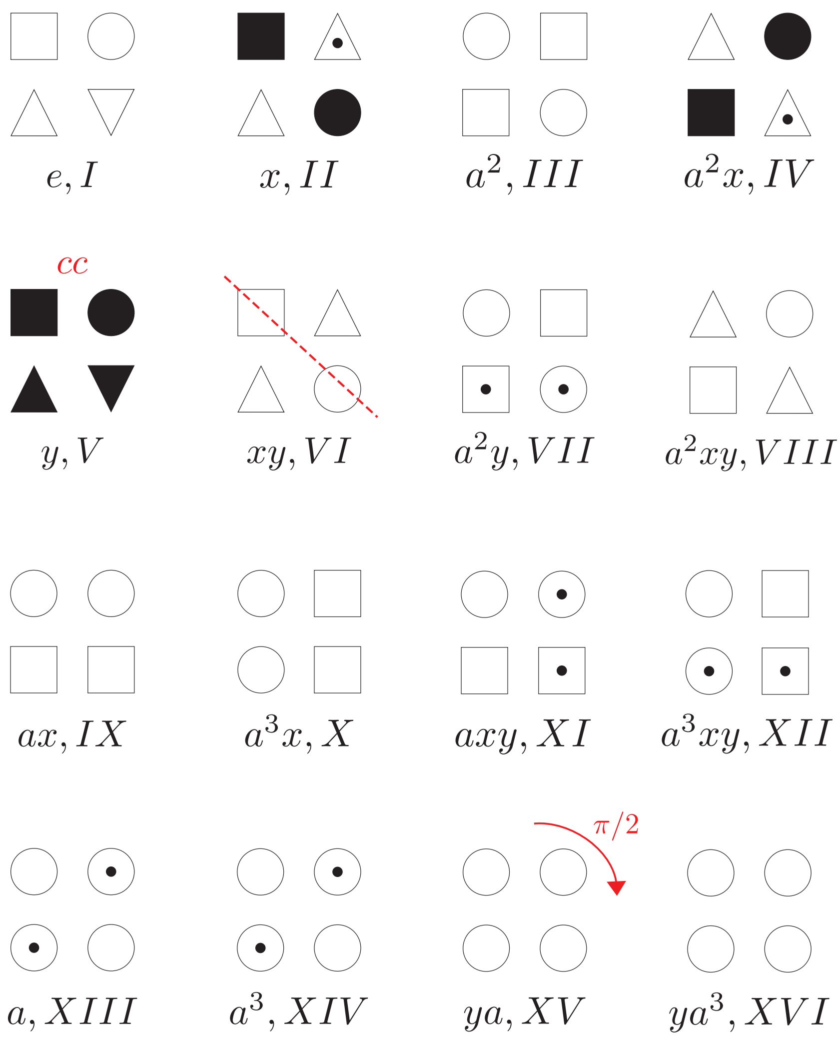

Figure 1. Representation of 2×2 matrices possesing the 16 symmetries compatible with G_{16}. The different symbols represent different complex numbers. The dotted symbols are complex conjugate of undotted ones. Filled symbols represent real numbers. The roman number and group-theoretical codes are displayed below each matrix. All symmetry operations can be constructed from three generators: among different choices we may use xy (flip along main diagonal), y (complex conjugation), and ya (rotation by $\pi/2$).

j runs from 1 to 16, the index k must jump among the 16 members of the group according to the multiplication table ($j \neq k$ except for $j = 1$ assigned to the identity). Since x is a symmetry of H, $\mathcal{S}_k H = \mathcal{S}_j H$, so that $\mathcal{S}_k \sim \mathcal{S}_j$ conditioned on $xH = H$. It might seem that we have 16 of these equivalence pairs. However, multiplying $\mathcal{S}_j x = \mathcal{S}_k$ by x from the right we find that $\mathcal{S}_j = \mathcal{S}_k x$. This means that there are in fact only eight equivalence pairs; in other words, the relations (pairs of equivalent operations) are always repeated once.

The only property of x we have used, apart from representing a symmetry, is $x^2 = 1$, so in general *any symmetry of H of order 2, implies eight pairs of equivalent superoperators*. Conditioned on $xH = H$, in particular, we find the equivalences

$$\begin{aligned} x \sim 1, ax \sim a, a^2x \sim a^2, a^3x \sim a^3, \\ ayx \sim ay, a^3yx \sim a^3y, yx^2 \sim xy, a^2yx \sim a^2y. \end{aligned} \tag{21}$$

Symmetry of order 4. Suppose now that H is invariant under a ($aH = H$). By applying a repeatedly we can create the subgroup of symmetries $\langle a \rangle$ in G_{SH}. Premultiplying the members of the group $\langle a \rangle$ by y, we get the set of superoperators ya, ya^2, ya^3, y. They are all equivalent,

$$yH = y(aH) = yaH = ayH, \tag{22}$$

$$yH = y(a^2H) = ya^2H = a^2yH, \tag{23}$$

$$yH = y(a^3H) = ya^3H = a^3yH. \tag{24}$$

The process may be repeated premultiplying the cyclic 4-group by 1, x and xy instead of y. Let us recall that the full group of 16 elements may be constructed by multiplying the cyclic group $\langle a \rangle$ by $\langle x, y \rangle$. Thus, this premultiplication of $\langle a \rangle$ by the elements of $\langle x, y \rangle = \{1, x, y, xy\}$ gives all 16 elements of the group G_{16} without repetitions. Each member of $\langle x, y \rangle$ produces an equivalent class of 4 elements, namely,

$$1, a, a^2, a^3, \tag{25}$$

$$x, xa, xa^2, xa^3, \tag{26}$$

$$y, ya, ya^2, ya^3, \tag{27}$$

$$xy, xya, xya^2, xya^3. \tag{28}$$

The first set of four elements is formed by symmetries of H while the others need not be symmetries. Also, multiplication in reverse order, i.e. $\langle a \rangle \times \langle x, y \rangle$ produces exactly the same equivalence classes because of the property $xa = a^3x$.

If a^3 is the assumed symmetry of H the same structure follows, since a^3 generates the same group of symmetries than a, namely $\langle a \rangle = \langle a^3 \rangle$.

When the other elements of order 4, ay and a^3y, are symmetries of H, they will also imply four sets of equivalent superoperators,

$$1, ay, a^2, ya^3, \tag{29}$$

$$x, xay, xa^2, xya^3, \tag{30}$$

$$y, y^2a, ya^2, a^3, \tag{31}$$

$$xy, xa, xya^2, xa^3, \tag{32}$$

where, as before, the first set corresponds to symmetries of H. The others may or may not be symmetries of H.

4.1.2. Consequences of two symmetries. Now suppose that the distinct superoperators $\mathcal{S}_i$ and $\mathcal{S}_j$ represent two symmetries of H. The consequences may be deduced by combining the results from the previous subsection. Let us first recall that the two symmetries may generate groups of two, four, and eight elements corresponding to symmetries as discussed in the previous section.

- The case corresponding to groups of two elements is trivial as it requires that one of the symmetries is the identity, and the other element should be of order 2. Therefore the discussion of the consequences has already been done in the previous subsection.
  In the following we assume that neither $\mathcal{S}_i$ nor $\mathcal{S}_j$ is the identity.
- A generated group of four elements $\langle \mathcal{S}_i, \mathcal{S}_j \rangle$ corresponds to commuting operations except the combination of an element of order 4 and an element not in the cyclic groups $Z4$. All elements of the generated group $\langle \mathcal{S}_i, \mathcal{S}_j \rangle$ will be symmetries of H. From there, the group table guarantees that it is always possible to find three other elements $\mathcal{S}_k$, $\mathcal{S}_l$, $\mathcal{S}_m$ such that the products $\mathcal{S}_n \langle \mathcal{S}_i, \mathcal{S}_j \rangle$, where $n = k, l, m$, define three classes of equivalent operations. They are equivalent, respectively, to $\mathcal{S}_k$, $\mathcal{S}_l$, and $\mathcal{S}_m$.
  Example: $\mathcal{S}_i = x$; $\mathcal{S}_j = y$. Then,
  $$\langle \mathcal{S}_i, \mathcal{S}_j \rangle = 1, x, y, xy \tag{33}$$
  is a group of symmetries of H. Choosing $\mathcal{S}_k = a$, $\mathcal{S}_l = a^2$, $\mathcal{S}_m = a^3$ we find the three sets of equivalent operations
  $$\begin{aligned} a, ax, ay, axy \\ a^2, a^2x, a^2y, a^2xy \\ a^3, a^3x, a^3y, a^3xy. \end{aligned} \tag{34}$$
- Finally, when $\langle \mathcal{S}_i, \mathcal{S}_j \rangle$ has eight elements, for example $\langle a, y \rangle$, or $\langle x, a \rangle$, the eight elements are symmetries of H, and *all other eight operations are equivalent to each other*. This is easy to prove. Multiplication of any element $\mathcal{S}_k$ not in $\langle \mathcal{S}_i, \mathcal{S}_j \rangle$ by the eight elements in $\langle \mathcal{S}_i, \mathcal{S}_j \rangle$ must produce eight distinct elements not in $\langle \mathcal{S}_i, \mathcal{S}_j \rangle$, because in the group table each element appears only once in any column (or row). These eight elements are all equivalent to $\mathcal{S}_k$.

4.1.3. Three or more symmetries. With three or more symmetries one may proceed similarly applying and combining the results of the previous two subsections. It is advisable to construct first the group generated by the three superoperators of the symmetries. Several combinations generate directly the whole group of 16 elements, for example x, y, and any element of order 4. Other sets of three elements generate subgroups of eight (for example $\langle x, y, a^2 \rangle$), or four elements (for example any three elements in a cyclic $Z4$ subgroup).

5. Implications of the symmetries on the eigenvalues.

If the Hamiltonian obeys a specific symmetry the eigenvectors and eigenvalues will fulfill certain conditions. For example, Hermitian Hamiltonians imply real eigenvalues, and Hamiltonians that commute with Π will have even or odd eigenvectors. A full and systematic analysis of the effect of all symmetries on the eigenvectors is out of the scope of the present work but we shall discuss here the effect of the symmetries on the energy spectra because of its physical relevance.

Let us first recall that the symmetries for which eigenvalues come in conjugate pairs E_j, E_j^* are symmetries II, IV, V, and VII, equivalently x, a^2x, y, and a^2y in group-theory notation. The reason for having conjugate pairs has been well discussed, see [13, 15–17], so we shall not insist on it further, except for recalling that the complex-pair condition implies the possibility to have real eigenvalues. While eigenvalues of Hermitian Hamiltonians ($xH = H$) are always real, the reality of eigenvalues for symmetries a^2x, y, and a^2y is not guaranteed, and requires specific parameter values, as discussed at length for PT-symmetry ($a^2yH = H$) since the seminal work [7].

We shall next pay attention to implications on the eigenvalues of the symmetries of order 4 in the two cycles $Z4$. For the other symmetries we have found no implications on the possible Hamiltonian eigenvalues, at least when they are the only symmetries.

5.1. a, a^3

Let as assume that $aH = H$, or, explicitly, that $H = H^\dagger\Pi$. Now we apply these operators on a right eigenvector of H,

$$H|E\rangle = E|E\rangle = H^\dagger|\Pi E\rangle. \tag{35}$$

Acting with $\langle E|$ from the left in the last equality,

$$E\langle E|E\rangle = E^*\langle E|\Pi|E\rangle. \tag{36}$$

The matrix elements on both sides are real. Now we make use of the fact that $a^2H = H$, or, translated into operators, $H = \Pi H\Pi$, i.e. H commutes with Π. For right eigenvectors with even or odd parity we find that

$$\text{If}\quad \Pi|E\rangle = |E\rangle \Rightarrow E\,\text{is real}, \tag{37}$$

$$\text{If}\quad \Pi|E\rangle = -|E\rangle \Rightarrow E\,\text{is imaginary}. \tag{38}$$

Of course the same splitting occurs when $a^3H = H$ since a and a^3 are associated symmetries.

5.1.1. ay, a^3y. We now assume that $ayH = H$, i.e. $\theta H^\dagger\Pi\theta = H$. Note that, as before, $a^2H = H$ holds as well automatically so that H commutes with Π. Making use of the ‘diagonal’ biorthogonal expression $H^\dagger = \sum|\widehat{E}\rangle E^*\langle E|$ (we omit subindices) one finds, similarly to the previous calculation

$$E^*\langle E|\theta|E\rangle = E^*\langle E|\Pi|\theta E\rangle, \tag{39}$$

which is now solved (assuming $\langle E|\theta|E\rangle \neq 0$) according to the two possibilities

$$\text{If}\quad \Pi|E\rangle = |E\rangle \Rightarrow E\,\text{is not restricted}, \tag{40}$$

$$\text{If}\quad \Pi|E\rangle = -|E\rangle \Rightarrow E = 0. \tag{41}$$

The same result holds for the associated symmetry $a^3yH = H$.

6. Discussion and conclusions

In this work we have explored the symmetry operations on, and symmetries possessed by, discrete (generally) non-Hermitian Hamiltonians. We have first seen that symmetry operations for discrete Hamiltonians are richer that for scattering Hamiltonians because they are not restricted by the properties of the kinetic energy. A non-Abelian group of 16 symmetry operations arises naturally represented by linear and antilinear superoperators that have geometrical interpretations in terms of the symmetry operations of the square and complex conjugation. A symmetry corresponds to the invariance of the Hamiltonian with respect to the transformation implied by one of these superoperators. We have studied the properties and structure of this group and also the implications of one or more existing symmetries in the rest of operations of the group, introducing the concepts of equivalent operations and of associated symmetries. The implications of some of these symmetries on the energy spectrum have also been discussed. While some of these symmetries have been extensibly studied, in particular PT-symmetry ($a^2yH = H$) [20], complex symmetric matrices ($xyH = H$) [21], and of course Hermitian matrices ($xH = H$), the broader frame introduced in this work provides a basis to relate, understand and exploit multiple symmetries and their interconnections. Combining discrete and continuous symmetry operations is also possible, as in [22, 23].

Some open questions and ideas for future work are: (i) to set the relation with optical systems or quantum optical systems and develop applications such as finding selection rules or device engineering. In particular physical realizations of non-Hermitian symmetries different from PT, e.g. with respect to a^2, xy, a^2xy, are doable in a quantum optical setting using two-level atoms interacting with a laser beam [5]. Our emphasis has been on Hamiltonians but general complex matrices of physical interest, such as a characteristic matrix of a stratified medium [24], are of course amenable to be transformed by operations in G_{16} and may posses some of the implied symmetries, e.g. with respect to a or a^3; (ii) To complete a systematic study of the effect of the 16 symmetries on right/left eigenvectors; (iii) To work out a 'representation theory' for non-Hermitian symmetries; iv) To extend the symmetries further. For example the symmetries described have their 'negative' versions in the form $\mathcal{S}H = -H$, or even more generally $\mathcal{S}H = \mathrm{e}^{\mathrm{i}\phi}H$, with ϕ being a real phase. In this regard it would be very interesting to relate the present work to the Bernard–LeClair symmetry classes of non-Hermitian random matrices and their variants [25, 26]. We just note at this point that some of the symmetries implied by G_{16} are not of the forms considered in [25].

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ORCID iDs

M A Simón https://orcid.org/0000-0001-6260-182X
J G Muga https://orcid.org/0000-0002-1967-502X

References

[1] Ruschhaupt A, Delgado F and Muga J G 2005 *J. Phys. A: Math. Gen.* **38** L171
[2] Longhi S 2017 *Europhys. Lett.* **120** 64001
[3] Konotop V V, Yang J and Zezyulin D A 2016 *Rev. Mod. Phys.* **88** 035002
[4] Feshbach H 1958 Unified theory of nuclear reactions *Ann. Phys., NY* **5** 357
[5] Ruschhaupt A, Damborenea J A, Navarro B, Muga J G and Hegerfeldt G C 2004 *Europhys. Lett.* **67** 1
[6] Muga J G, Palao J P, Navarro N and Egusquiza I L 2004 *Phys. Rep.* **395** 357
[7] Bender C M and Boettcher S 1998 *Phys. Rev. Lett.* **80** 5243

[8] Nixon S and Yang J 2016 *Phys. Rev.* A **93** 031802
[9] Nixon S and Yang J 2016 *Opt. Lett.* **41** 2747
[10] Chen P and Chong Y D 2017 *Phys. Rev.* A **95** 062113
[11] Ruschhaupt A, Dowdall T, Simón M A and Muga J G 2017 *Europhys. Lett.* **120** 20001
[12] Simón M A, Buendí a A and Muga J G 2018 *Mathematics* **6** 111
[13] Simón M A, Buendía A, Kiely A, Mostafazadeh A and Muga J G 2019 *Phys. Rev.* A **99** 052110
[14] Mostafazadeh A 2010 *Int. J. Geom. Methods Mod. Phys.* **07** 1191
[15] Mostafazadeh A 2002 *J. Math. Phys.* **43** 205
[16] Mostafazadeh A 2002 *J. Math. Phys.* **43** 2814
[17] Mostafazadeh A 2002 *J. Math. Phys.* **43** 3944
[18] Wigner E P 1959 *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra* (New York: Academic) pp 233–6
[19] Zee A 2016 *Group Theory in a Nutshell for Physicists* (Princeton, NJ: Princeton University Press)
[20] Znojil M 2015 *Non-Selfadjoint Operators in Quantum Physics* ed F Bagarello *et al* (Hoboken, NJ: Wiley) ch 1 p 7
[21] Garcia S R, Prodan E and Putinar M 2014 *J. Phys. A: Math. Theor.* **47** 353001
[22] Kartashov Y V, Konotop V V and Zezyulin D A 2014 *Europhys. Lett.* **107** 50002
[23] Zezyulin D A, Kartashov Y V and Konotop V V 2017 *Opt. Lett.* **42** 1273
[24] Born M and Wolf E 1999 *Principles of Optics* 7th edn (Cambridge: Cambridge University Press) p 63
[25] Bernard D and LeClair A 2002 A classification of non-Hermitian random matrices *Statistical Field Theories* (*NATO Science Series* vol 73) ed A Cappelli and G Mussardo (Dordrecht: Springer) pp 207–14
[26] Kawabata K, Shiozaki K, Ueda M and Sato M 2019 *Phys. Rev.* X **9** 041015